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# Comparison of the Toxicity of the Combustion Products From A Flexible Polyurethane Foam and A Polyester Fabric Evaluated Separately and Together By the NBS Toxicity Test Method and A Cone Radiant Heater Toxicity Test Apparatus

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U.S. DEPARTMENT OF COMMERCE  
National Bureau of Standards  
Center for Fire Research  
Gaithersburg, MD 20899

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**U.S. DEPARTMENT OF COMMERCE, Malcolm Baldrige, *Secretary***  
**NATIONAL BUREAU OF STANDARDS, Ernest Ambler, *Director***



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COMPARISON OF THE TOXICITY OF THE COMBUSTION PRODUCTS FROM A FLEXIBLE  
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AND TOGETHER BY THE NBS TOXICITY TEST METHOD AND A  
CONE RADIANT HEATER TOXICITY TEST APPARATUS<sup>1, 2</sup>

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ABSTRACT

Representative specimens of flexible polyurethane foam and polyester fabric were thermally decomposed separately and together in order to compare the toxicity of the combustion products from the combined materials with those from the single homogeneous materials and to compare the toxicological results obtained with the NBS Toxicity Test Method with those using a cone radiant heater toxicity test apparatus. Gas concentrations (CO, CO<sub>2</sub>, O<sub>2</sub> and HCN), blood carboxyhemoglobin, and LC<sub>50</sub> values in Fischer 344 rats were determined for the separate and combined materials under both flaming and non-flaming conditions. Using the NBS Toxicity Test Method, the non-flaming combined experiments indicated that both materials contributed in an additive manner to the concentration of the combustion products. However, under flaming conditions, the generation of HCN is greater than that predicted from the addition of the maximum amounts produced by the materials separately. With the cone radiant heater apparatus operated so as to generate the maximum concentrations of combustion products in the animal exposure chamber, deaths were observed in the combination experiments, but not in the single material exposures. In the combined material testing with both toxicity test systems, flaming conditions produced deaths within the 30 minute exposures; whereas, non-flaming conditions produced deaths following the exposures. Estimated LC<sub>50</sub> values for the combined materials in the radiant furnace were not greatly different from the calculated values obtained with the NBS Toxicity Test.

Key words: combustion products; inhalation; lethal concentrations; Toxicity Test Methods; polyesters; polyurethane foams; radiant heat; toxicity; upholstered furniture.

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## 1. INTRODUCTION

The United States has the worst fire loss record in the industrialized world [1]<sup>4</sup>. The fire scenario which produces the most fire deaths in the U.S. begins with an inadvertently dropped cigarette in an upholstered chair, which smolders for an undetermined time period (sometimes more than an hour) before bursting into flames. Approximately 2/3<sup>rds</sup> of all fire deaths occur away from the room of fire origin and many of the victims of such fires die of smoke inhalation in or near their beds indicating little or no attempt or ability to escape.

Since the majority of commercially available upholstered furniture today contains flexible polyurethane foam as a filling material and a covering fabric which is either a cellulosic or a thermoplastic (such as polyester), polyurethane and polyester were chosen for this study. Many small-scale laboratory studies have examined the toxicity of the combustion products from either flexible polyurethane foams [2] or polyesters [3]. There have also been numerous large-scale room burns of chairs, multiple materials, or composite materials which have included among others, flexible polyurethane foams and polyesters. However, to our knowledge, there has been no systematic study which has examined the acute inhalation toxicity of the thermal degradation products from combinations of materials, first as separate materials and then together as is reported here.

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<sup>4</sup> Numbers in brackets refer to the literature references listed at the end of this report.

Experiments by Alarie et al. were somewhat similar in concept in that they compared the toxicity of individual materials (determined in small-scale tests) with the toxicity of multiple combined materials (determined in large-scale chair burns) [4]. However, the objective of their study was to compare the toxicity of the combined major components of the chairs (flexible polyurethane foam, polyester, and cotton fiber) with their individual toxicities in small-scale tests. They did not study the toxicity of the combined components in the small-scale tests.

This study was designed to examine: (a) the toxicological effects from the combustion products of a flexible polyurethane foam and a polyester fabric (alone and in combination) in order to determine the contribution of each material to the overall toxicity of the mixture and (b) to compare the toxicological results obtained under the conditions of the NBS Toxicity Test Method [5] with those from a radiant cone heater toxicity test apparatus [6]. Three separate aspects of testing composite materials were considered: (1) Are the results for the composite specimen derivable from mass-proportioning the component results or does some unexpected toxicological interaction occur? (2) Would the yields of the major toxicants be affected? (3) Are the observed lethalties predictable based on the individual or combined concentrations of the primary toxic gases, namely, carbon monoxide (CO), carbon dioxide (CO<sub>2</sub>), and hydrogen cyanide (HCN)?

## 2. MATERIALS AND METHODS

### 2.1 Materials

The materials studied were a polyester upholstery fabric (100% polyester, scoured and dyed dark blue) and a flexible polyurethane foam, two common components of commercially available upholstered chairs. Both materials were obtained from the Consumer Product Safety Commission, Washington, D.C. 20207 and were generically classified, i.e., the specific chemical formulations were unknown. The results of a previous toxicological study on the same polyurethane foam, designated CPSC #13, have been published [7].

### 2.2 Chemical Analysis

Carbon monoxide and CO<sub>2</sub> were measured continuously by non-dispersive infrared spectroscopy. Oxygen (O<sub>2</sub>) concentrations were measured continuously by a galvanic cell or a paramagnetic analyzer. The CO, CO<sub>2</sub>, and O<sub>2</sub> data were recorded by an on-line computer controlled data collection system every 15 seconds. Hydrogen cyanide was sampled with a gas-tight syringe approximately every three minutes and analyzed with a gas chromatograph equipped with a thermionic detector [8].

### 2.3 Animals

The animals used for these experiments were Fischer 344 male rats weighing 200-300 grams. They were obtained from the Harlan Sprague-Dawley Company

(Walkersville, Maryland)<sup>5</sup> or Taconic Farms (Germantown, New York) and were allowed to acclimate to our laboratory conditions for at least 10 days prior to experimentation. Animal care and maintenance were performed in accordance with the procedures outlined in the National Institutes of Health's "Guide for the Care and Use of Laboratory Animals" [9]. Each rat was housed individually in suspended stainless steel cages and provided with food and water ad libitum. Twelve hours of fluorescent lighting per day were provided using an automatic timer. All animals were weighed daily from the day of arrival until the end of the post-exposure observation period. Control animals from the same batch were weighed daily also.

#### 2.4 Animal Exposures

Twenty-four hours prior to the exposures, one or two animals per experiment were anesthetized with nembutal and cannulated. This procedure involved the surgical insertion of a cannula into the animal's femoral artery [10], thereby allowing blood samples to be taken before and during the exposure from unanesthetized animals. The blood levels of COHb are indicative of the amount of carbon monoxide inhaled by the animals.

Six rats were exposed in each experiment. Each rat was placed in a restrainer which was then inserted into one of the six portholes located along the front

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<sup>5</sup> Certain commercial equipment, instruments, materials or companies are identified in this paper in order to adequately specify the experimental procedure. In no case does such identification imply recommendation or endorsement by the National Bureau of Standards, nor does it imply that the equipment or material identified is necessarily the best available for the purpose.

of the exposure chamber such that only the heads of the animals were exposed to the combustion atmospheres. Exposures were for 30 minutes, during which time heparinized blood samples were taken prior to, approximately 15 minutes into, and just before the end of the experiment from the cannulated animals.

The toxicological endpoint was death. The number of animals that died at each mass loading of material was plotted to produce a concentration-response curve, from which an  $LC_{50}$  (30 minutes and 14 days) value was calculated. The  $LC_{50}$  was defined as the mass loading of material per unit chamber volume (mg/l) which caused 50% of the animals to die during the 30 minute exposure plus the post-exposure observation period. In this series of experiments, animals that were still losing weight on day 14 were kept until they died or recovered as indicated by three days of successive weight gain. These animals that died after day 14 were also included in the  $LC_{50}$  calculation. The  $LC_{50}$ 's and their 95 percent confidence limits were calculated via the statistical method of Litchfield and Wilcoxon [11].

## 2.5 The NBS Toxicity Test Method

In the first part of this study, the acute inhalation toxicity of the combustion products from the test materials was evaluated according to the NBS Toxicity Test Method [5]. Briefly, the test method consists of three major components: (1) a combustion system, (2) a chemical analysis system (see section 2.2), and (3) an animal exposure system (see section 2.4) (Fig. 1). The entire system is a closed design in which all the combustion products are generated in a 1000 ml quartz cup furnace located directly below the 200 liter

PMMA rectangular exposure chamber (Fig. 2) and are kept within the chamber except for the volume which is transferred for chemical analysis and subsequently returned. Temperature measurements in the cup furnace and at animal exposure positions #1, 3, and 6 are measured continuously and recorded every 15 seconds by an on-line computer controlled data collection system.

The cup furnace is similar to that designed by Potts and Lederer (Fig. 3) [12]. Each material is evaluated under separate flaming and non-flaming conditions in which the cup furnace is preset at 25°C above or below the material's autoignition temperature, respectively. The autoignition temperature, in this case, is defined as that temperature which causes the sample to flame spontaneously during a 30 minute exposure. In the actual flaming exposures, ethanol and/or an electric spark are used to ensure immediate flaming.

For this series of tests, additional experiments at temperatures other than the standard ones (i.e., 25°C above and below the autoignition temperatures) were necessary to estimate the toxicological contribution of each material when tested in combination with the other. Therefore, the toxicity and test atmospheric gases (CO, CO<sub>2</sub>, HCN and O<sub>2</sub>) from the polyester were also examined at the non-flaming temperature of the polyurethane foam (375°C) and the test atmospheric gases produced from the thermal decomposition of flexible polyurethane foam were measured at the flaming temperature of the polyester (525°C).

Combinations of the polyester and the polyurethane foam were thermally decomposed in the cup furnace at a non-flaming temperature of 375°C (which was

the temperature at which the polyurethane foam was examined in the non-flaming mode and the highest possible non-flaming combination test temperature, since the polyurethane foam would flame at higher temperatures) and a flaming temperature of 525°C (the temperature at which both the polyurethane and polyester would undergo flaming combustion, if tested separately).

According to the NBS Toxicity Test Method, the highest concentration of material tested should not exceed 40 mg/l. However, to complete this series of experiments, especially those tests with combined materials, it was sometimes necessary to exceed this limit. If no deaths occurred at the highest concentration tested, the LC<sub>50</sub> is listed as greater than that concentration.

## 2.6 Experimental Procedure with the NBS Toxicity Test Method

Prior to each experiment, the quartz cup from the furnace was weighed. The furnace was preset to the desired temperature for the non-flaming or flaming exposures. The material was cut to the desired weight and control blood was taken from the cannulated animals. The animals in their restrainers were placed into the front portholes in the exposure chamber. The experiments began when the material was dropped into the heated cup and the door to the chamber closed. Blood samples were taken during the 30 minute exposures and the animals were observed to determine time of death as indicated by lack of respiration. At the end of the exposures, the animals were removed, checked for various physiological and behavioral functions, such as eye reflexes, nasal and mouth discharges, breathing rate, righting reflexes, posture, and exploratory behavior. Cannulated animals were sacrificed and not kept for the

post-exposure observation period. Animals sacrificed immediately following the exposures were not counted in the  $LC_{50}$  calculations based on the 30 minute and 14 day post-exposure periods. If  $LC_{50}$  calculations were made based only on deaths occurring during the 30 minute exposures, the cannulated animals were counted. All surviving animals were replaced in their cages and weighed daily for at least 14 days as noted above. The cup and residues were removed from the hot furnace, allowed to cool, and weighed to determine the mass of material consumed during the exposures. This information allows one to calculate the  $LC_{50}$  values based on amount consumed per chamber volume in addition to that based on the amount loaded, if desired.

## 2.7 The Cone Radiant Heater Toxicity Test Apparatus

The cone radiant heater toxicity test apparatus (Fig. 4) was similar to the NBS Toxicity Test Method in that it consisted of three components: 1. an animal exposure system, 2. a chemical analytical system and 3. a combustion system. The animal exposure and the chemical analytical systems were essentially the same as those utilized in the NBS method with the following exceptions: the animal exposure chamber was the same size (200 l) and shape (rectangular), but was constructed of 25 mm thick PMMA instead of 12 mm in order to maintain a vacuum. It was also reinforced with polytetrafluoroethylene-coated steel supports. The animals received square-wave exposures to the test atmospheres rather than being inserted first and experiencing the initial thermal decomposition products of the materials. As in the NBS method, continuous gas analysis was performed to monitor the concentrations of CO, CO<sub>2</sub>, and O<sub>2</sub> in the animal exposure chamber during the 30 minute animal exposures. However, in

this case, because the animal exposure chamber was designed to be evacuated prior to each experiment, the gas sampling line was equipped with a dead space sampling loop that allowed for the intermittent gas sampling for HCN. A thermocouple was installed in one of the pipe fittings to ensure that the animal exposure chamber temperature was below the maximum allowable temperature of 40°C before the animals were inserted.

The major difference between the two apparatuses was in the combustion systems. Instead of a 1000 ml quartz cup furnace located below the animal exposure chamber, the furnace consisted of a cone radiant heater enclosed in a separate 100 l pyrex combustion chamber. Below the cone heater, a load cell was mounted to continuously monitor the sample weight loss during an experiment. Air flow through the combustion chamber was controlled by metering compressed gases into the bottom of the chamber. The combustion atmosphere was transferred from the combustion chamber through a square pyramid-shaped hood to a horizontal exhaust duct (114 mm I.D.); a portion of this combustion atmosphere was drawn through a 9 mm I.D. stainless steel sampling line to the animal exposure chamber and the rest escaped through a main exhaust duct. The sampling line to the animal exposure chamber was connected to a ball valve which manually controlled the gas flow rate between the combustion chamber and animal exposure chamber. A differential pressure transducer was connected to two points along a straight section of the sampling line to allow for the actual measurement of flow rate into the animal exposure chamber.

The cone radiant heater was similar in design to the heater used with the Cone Calorimeter (Fig. 5) [13] and the ISO heater [14]. The heater was constructed

of a double wall (to minimize heat radiation to the outside wall) and contained a heater element of coiled resistance heating wire packed in magnesium oxide refractory and covered with a high temperature alloy sheath. The power to the heater was controlled by a closed loop electronic controller connected to three thermocouples located behind the coil windings. The heater could be set to apply a relatively uniform radiation field over the sample surface from 0 to 11 W/cm<sup>2</sup>.

## 2.8 Experimental Procedure Using the Cone Radiant Heater Apparatus

Prior to testing, the autoignition heat flux for each material was determined by exposing a series of specimens to different incident heat flux levels and noting the minimum heat flux necessary to cause a sample to self-ignite. In general, if a specimen had not self-ignited within ten minutes, the incident heat flux level was increased. Actual testing was conducted with the incident heat flux level set slightly below the autoignition heat flux. This produced a non-flaming exposure. In the flaming experiments, an AC electric spark discharge was used to assure flaming once surface decomposition was sufficient to develop a flammable mixture above the sample surface. This induction period was short (5-15 seconds) for these materials.

Before each experiment, the combustion and exposure chambers as well as the sampling pipe and control valve connecting the two chambers were cleaned. The cleaning of the latter two items was necessary to prevent clogging of components. The specimen material was cut to the proper dimensions - a face size of 100 mm by 100 mm. The depth of the specimen varied with the test

material. When tested in combination, 76 mm of foam were covered on the top and sides with one layer of fabric.

At the beginning of each test, an airflow rate through the combustion chamber was selected. The cone heater was adjusted to the proper height to ensure that the upper sample surface would be at the correct distance from the cone heater. Power was applied to the cone heater and the heater controller was set to maintain the cone heater at a constant temperature. A water cooled heat flux meter was used to measure the actual heat flux incident on the sample surface. When the cone heater was stabilized at a desired energy level, the heat flux meter was removed.

While the cone heater was reaching equilibrium, the exposure chamber was sealed at all openings. The inlet control valve was shut, and the analyzer lines and the animal ports were closed. The exposure chamber was evacuated to approximately 3 kPa or less of pressure.

The tests began when the material sample was placed below the cone radiant heater on the load cell in the combustion chamber and the data acquisition started. With the exhaust damper control opened approximately 40%, the sample was allowed to decompose. Depending on the combustion mode, flaming or non-flaming, transfer of the duct gases into the animal exposure chamber began two to four minutes after the start of the sample exposure.

The animal exposure chamber was filled at a rate that was less than the combustion chamber airflow rate. This sampling rate was maintained constant

throughout the filling process by means of a manual control, using the differential pressure gage. Since the filling process was driven solely by the pressure difference between the evacuated animal chamber and the essentially atmospheric pressure combustion chamber, complete filling with combustion products would take an infinite period of time. Instead, when the chamber was filled to a pressure of 95 kPa with combustion products, the control valve was shut. The exposure chamber was then filled to atmospheric pressure by introducing clean air from a supply tank.

When the exposure chamber reached atmospheric pressure, the gas analyzers were connected to the exposure chamber. The animal chamber temperature was noted to assure that it was below the maximum value (40°C) permitted for the animals. (It was possible to wait until the gases cooled before inserting the animals.) The animals were then inserted simultaneously into the portholes along the front of the animal chamber and received 30 minute square-wave exposures to the test atmospheres. Treatment of the animals prior, during and following the exposures were similar to that received during the NBS Toxicity Test.

## 2.9 Data Reduction for the Cone Radiant Heater Test Apparatus

The mass consumed (i.e., pyrolysate concentration) and transferred to the animal exposure chamber, in units of mg/l, was computed assuming:

- instantaneous mixing of the pyrolysate in the combustion chamber; and
- no material loss on the interior surfaces of the combustion chamber, exhaust duct, connecting pipe, and animal exposure chamber.

The latter assumption was found not to be strictly valid. Following each test, the control valve between the combustion chamber exhaust duct and the animal exposure chamber was disassembled and cleaned. Significant quantities of soot and tar were observed to have deposited on the surfaces of the control valve orifice and the upstream pipe leading from the exhaust duct to the control valve. However, in these experiments, these losses could not be quantified. Therefore, the calculated concentration values in mg/l reported in Tables 4, 5, and 6 represent upper limit concentrations. The actual exposure concentrations were less than the tabulated values.

A complete derivation of the solution of the relevant differential equations used to calculate the pyrolysate concentration to which the animals were exposed in each experiment is given in Appendix A. For the sake of simplicity, the material loss response to a given external radiant energy field was divided into a series of straight line segments. For a constant volumetric air flow through the combustion, the exhaust material concentration was calculated for each time segment. It was assumed that the animal exposure box was being filled at the same concentration. For each experiment, the sampling flow rate from the exhaust duct into the exposure chamber was constant as described above.

### 3. RESULTS

#### 3.1 The NBS Toxicity Test

##### 3.1.1 Flexible Polyurethane Foam

The autoignition temperature of the polyurethane foam used in these experiments was 400°C. The chemical and toxicological data obtained from the flexible polyurethane foam thermally decomposed in both the non-flaming (375°C) and flaming (425°C) modes according to the NBS Toxicity Test Method are presented in Table 1. This table also provides the chemical results obtained when the polyurethane was degraded at 525°C, the flaming temperature at which polyester was tested. In both the non-flaming and flaming modes, the residues consisted of black light-weight chars.

Similar to other non-fire retarded flexible polyurethane foams tested in this laboratory, no animal deaths occurred during the 30 minute exposures regardless of the concentration (up to 40 mg/l) of the polyurethane or the mode of decomposition - non-flaming or flaming [5,7]. Deaths were only noted during the 14 day observation period following exposure to the non-flaming combustion products (Fig. 6). The  $LC_{50}$  value for the non-flaming mode was 37.0 mg/l with 95% confidence limits of 29.8 - 46.0 mg/l. The  $LC_{50}$  value for the flaming mode was greater than 40 mg/l, i.e., no animal deaths were noted either within or post-exposure from any of the concentrations (up to 40 mg/l) tested.

### 3.1.2 Polyester

The autoignition temperature of the polyester fabric was 500°C. Therefore, the polyester fabric was tested in the flaming mode at 525°C and in the non-flaming mode at two temperatures: 475°C (25°C below its autoignition temperature) and 375°C (the non-flaming decomposition temperature of the polyurethane foam). The residue from the flaming and non-flaming thermal decomposition of the polyester was also black but appeared heavier than that of the polyurethane and looked like the remains of the melted sample. The chemical and toxicological data collected from the thermal degradation of polyester by the NBS test method are shown in Table 2.

In the non-flaming mode at 475°C, the LC<sub>50</sub> value of the polyester was 39.0 mg/l with 95% confidence limits of 38.4 - 39.5 mg/l (Fig. 7 & 8). Animal deaths were noted both during and following the 30 minute exposures. At decomposition temperatures 100°C lower (375°C), no animal deaths were observed at any time. Therefore, the LC<sub>50</sub> value at 375°C is given as greater than 50 mg/l, which was the highest mass of material/chamber volume tested. However, it is important to note that at the lower temperature (375°C), only 22-55% of the original sample was consumed; whereas, at 475°C, approximately 85% of the sample was consumed. Based upon a comparison of the toxicological effects at the actual masses consumed at 475°C, deaths would not be expected at the masses consumed at the lower temperature.

In the flaming mode, deaths occurred both during and following the exposures. Based on mass of material loaded per chamber volume, the  $LC_{50}$  value for the 30 minute exposure and 14 day post-exposure period was 37.5 mg/l with 95% confidence levels of 35.3 - 39.8 mg/l (Fig. 8).

### 3.1.3 Flexible Polyurethane Foam and Polyester Combined

#### 3.1.3.1 Non-Flaming Combined Experiments

The thermal decomposition of both flexible polyurethane foam and polyester in the non-flaming mode was studied at 375°C which was 25°C and 125°C below the autoignition temperatures of the polyurethane and the polyester, respectively. In most of these experiments, the polyester fabric was folded and dropped into the cup furnace immediately preceding the polyurethane foam. In two experiments, to be discussed later, the polyurethane foam was covered by the polyester fabric. Upon heating, the samples collapsed in less than one minute and formed a black ball in approximately two minutes.

Since the polyester smoke was not toxic at 375°C even at the highest loading tested (50 mg/l), a sublethal amount of polyester (20 mg/l) was chosen to test whether this addition would increase the toxicity (lethality) of the polyurethane foam in the combination experiments. If the polyester component has no effect at this temperature, then the addition of 20 mg/l of polyester to the  $LC_{50}$  value of the polyurethane (37 mg/l) should increase the  $LC_{50}$  value of the mixture by 20 mg/l to 57 mg/l (Fig. 9). The results, however, showed that the

LC<sub>50</sub> value of the combined materials only increased to 47.5 mg/l, an indication that the polyester is contributing to the toxicity by about 10 mg/l (Table 3). Since a significant proportion of the polyester is not decomposed at 375°C, these data were also analyzed on the basis of mass consumed/chamber volume. The experiments on the polyester at 375°C showed that when 3.88 grams (20 mg/l) were loaded into the cup furnace, 78% remained as residue and only 4.3 mg/l were actually consumed. According to the same reasoning used before, that is, under the assumption that the polyester at this temperature has no effect on the combined toxicity, then the LC<sub>50</sub> of the mixture of polyurethane (with an LC<sub>50</sub> of 31.9 mg/l, consumed weight) and polyester (a "non-toxic" amount of 4.3 mg/l, consumed) should increase by 4.3 mg/l producing a combined LC<sub>50</sub> of 36.2 mg/l. However, the LC<sub>50</sub> of the combination is only 26.2 mg/l, consumed weight, indicating that the polyester increases the toxicity by about 10 mg/l (i.e., 36.2 minus 26.2 mg/l); this is the same increase calculated when the mass loaded, rather than mass consumed, was considered.

Two experiments were conducted to test the effect of covering the foam with the polyester. In these cases, 47.5 mg/l of the polyester fabric were needed to cover the polyurethane. The results of these experiments indicated that there was too much material in the furnace (i.e., the system was overloaded) to produce accurate results (Table 3). Indications of the overload were (1) an increase in the mass loaded in the furnace did not increase the mass consumed, (2) the concentrations of CO and CO<sub>2</sub> decreased with increasing mass, and (3) the mortalities were fewer at the higher material loadings.

In those non-flaming experiments in which 20 mg/l of polyester were added to different loadings of flexible polyurethane foam, all deaths occurred during the post-exposure period and none occurred during the 30 minute exposures. These results are more characteristic of the experiments on polyurethane decomposed by itself and different from those seen with the polyester alone. No deaths were observed during exposure even when the polyester loading was increased to 47.5 mg/l in the two experiments designed to test the effect of decomposing polyurethane completely covered with polyester fabric (Table 3).

#### 3.1.3.2 Flaming Combined Experiments

The experiments in which the flexible polyurethane foam and polyester were combined and tested in the flaming mode were conducted at 525°C (25°C above the autoignition temperature of the polyester) to ensure that both materials would flame. A black residue was noted at the end of the 30 minute exposures.

In these experiments, the mass loading of polyurethane was kept constant at 3.88 grams (20 mg/l) and only that of the polyester was varied (Table 3). The reason for this approach was the same as for the non-flaming experiments, i.e., to see if a non-lethal amount of the less toxic material (in this case, the polyurethane foam) would increase the toxicity of the polyester whose LC<sub>50</sub> could be measured. The polyurethane foam when tested by itself in the flaming mode at 425°C had produced no deaths either during or post-exposure at concentrations up to 40 mg/l (Fig. 10); whereas, the polyester fabric, when decomposed by itself in the flaming mode at 525°C, had produced both within and post-exposure deaths. The LC<sub>50</sub> value for the flaming polyester fabric by

itself was 37.5 mg/l. Therefore, if the polyurethane was toxicologically inert, the addition of 20 mg/l of polyurethane should have raised the LC<sub>50</sub> value of the mixture to 57.5 mg/l. In actuality, the 30 minute and 14 day LC<sub>50</sub> value calculated for the combined exposures was 39.0 mg/l with 95% confidence limits of 36.0 - 42.2 mg/l. These results, showing that the LC<sub>50</sub> value for the combined materials was lower than expected by almost the exact amount of polyurethane added to the system, are an indication that the polyurethane and the polyester are both contributing to the toxicity in an additive manner. However, since all of the deaths occurred during the exposures, the results of these experiments more closely resemble those of the polyester tests rather than those of the polyurethane experiments.

Another way to examine these data is to look at the toxic effects of the individual components of the mixture. For example, in one of the flaming experiments shown in Table 3, 20 mg/l of the flexible polyurethane foam plus 20 mg/l of the polyester caused the deaths of 50% of the test animals; whereas, 20 mg/l of the polyurethane foam decomposed by itself in the flaming mode produced no deaths (Table 1) and the polyester decomposed by itself did not produce any deaths below a concentration of 35 mg/l (Table 2). Thus individual sublethal concentrations of this polyurethane foam and polyester fabric were adding up to a concentration which was lethal.

## 3.2 The Radiant Cone Heater Toxicity Test Apparatus

### 3.2.1 Flexible Polyurethane Foam

The radiant flux at which the polyurethane foam would spontaneously ignite was found to be  $2.08 \text{ W/cm}^2$ . The non-flaming and flaming experiments were, therefore, conducted at  $2.0 \text{ W/cm}^2$ . Flaming was initiated by an electrical spark. The experimental conditions, i.e., air flow, mass loaded, and gas sampling times (times during which the animal exposure chamber was filled with combustion products), and the experimental results, i.e., mass consumed, gas concentrations in the animal exposure chamber, and toxicological data are given in Table 4. The conditions were varied in order to generate the most toxic atmospheres. For example, the maximum amount of sample was loaded into the furnace and the air flow rates through the combustion chamber were reduced as low as possible to minimize dilution effects. Regardless of the conditions, however, no animals died either during or following the non-flaming or flaming exposures.

### 3.2.2 Polyester Fabric

The radiant flux at which the polyester fabric would spontaneously ignite was determined to be  $4.0 \text{ W/cm}^2$ . The non-flaming exposures were performed at  $2.0 \text{ W/cm}^2$  which was the same radiant heat used for the examination of the polyurethane. The flaming exposures were performed at  $3.5 \text{ W/cm}^2$  and flaming was initiated by an electrical spark. Again, the experimental conditions were

maximized to produce the most toxic atmospheres. Table 5 gives the results of the polyester experiments.

The maximum concentrations of gases transferred to the animal exposure chamber under the non-flaming conditions were so low (approximately 100 ppm of CO and 650 ppm of CO<sub>2</sub>), that it was deemed futile to expose animals. The exposure chamber concentration of combustion products was calculated to be equivalent to a mass consumed of <5 mg/l and since this was considered the maximum amount possible, no further non-flaming experiments were performed.

The maximum amounts of gases generated under flaming conditions were higher than in the non-flaming experiment and the concentrations transferred to the exposure chamber were about 1900 ppm of CO and 5% CO<sub>2</sub>. This combustion atmosphere was also not sufficient to cause any deaths either within or following the exposure.

### 3.2.3 Combined Polyurethane and Polyester Experiments

These experiments were conducted with polyester-covered polyurethane foam samples exposed to a radiant flux of 2.0 W/cm<sup>2</sup>. Again, conditions were maximized to try to produce the most toxic exposure chamber environments (Table 6). In the non-flaming mode, no animals died during the exposures, but 3/6 died during the post-exposure observation period. Two died during the 14 days and one died on day 25. A repeat of the same experiment, but with a reduced air flow rate through the combustion chamber (which should have increased the toxicity), produced no animal deaths.

In the flaming mode, the worst case conditions produced 5/6 animal deaths during one experiment and no post-exposure deaths. An attempt to replicate the same experiment resulted in no deaths (Table 6). The reasons for the lack of replication are unclear at this time.

#### 4. DISCUSSION

A flexible polyurethane foam and a polyester fabric were thermally decomposed separately and together in order to examine and compare the toxicity from the single homogeneous materials and mixtures of the two using both the NBS Toxicity Test Method and a cone radiant heater toxicity test apparatus.

The cone radiant heater toxicity apparatus was designed to explore the toxicological effects of a variety of possible combustion environments needed in order to expose non-uniform materials under normal performance conditions typifying end use. Furniture composites, wall material composites, and composite reinforced plastics have been satisfactorily tested in the Cone Calorimeter for heat, smoke, and gas generation rates [13]. This capability was considered an operational advantage of the cone radiant heater over the cup furnace. However, the following limitations, not present in the cup furnace apparatus, were found for the cone heater apparatus when used as a combustion source in connection with a static animal exposure system:

- Determinations of the concentration of combustion products in the animal exposure chamber. Difficulties arose in transferring a representative sample and sufficient quantity of combustion products from the combustion chamber to the animal exposure chamber. Another problem was the determination of the mass of thermally decomposed material which represented the amount of combustion products actually transferred to the exposure chamber (see Appendix A).
- Transfer line clogging. The transfer line clogged badly due to soot deposition. It was not considered desirable to filter or otherwise eliminate the soot since this could selectively remove toxicants and result in decreasing the measured effluent toxicity. The amount of deposition required that the line be disassembled after every test, cleaned out, and reassembled. It also meant that toxic products might not be reaching the animals. This deposition might have been lessened by heating the line, since a portion of such wall losses are due to condensation and thermophoretic effects, which would be eliminated if the line temperature were kept above the gas temperature. However, since part of the line was located inside the combustion chamber, since a control valve was involved, and since the animal chamber temperatures could be adversely affected, the design of a proper line heater became quite difficult and was not undertaken. The decomposition of soot in the stack between the combustion chamber and the sampling line also posed the problem of potential carry-over of toxicants from one test to another, especially if the testing mode changed from non-flaming to flaming.

- Filling rate control. The filling rate was controlled by monitoring the differential pressure across a length of transfer line, and using the manual control valve to maintain this pressure at a level corresponding to a uniform filling rate. The relationship between the pressure readings and the filling rate was pre-determined from flow calibrations. In some cases, good control was difficult to achieve under all conditions, i.e., both with the animal chamber evacuated and with the chamber nearly back-filled. A mass flow controller was considered but was not implemented because significant difficulties were expected from sooting.
- Large reservoir volume in the combustion chamber. The Pyrex-enclosed combustion chamber represented a substantial volume of approximately 100ℓ if the exhaust piping up to the stack control valve was included. The mixing and dilution of the combustion products with this volume of initially ambient air would not be a problem if combustion rates and flow rates of the air were rapid. In the case of low density foam, however, only a small amount of specimen mass was available. Therefore, very small combustion chamber air flow rates had to be set. Under these conditions, there was a substantial error in determining the concentration of combustion products in the combustion chamber, and, consequently, in the equivalent mass loading needed to calculate the  $LC_{50}$ . Also, any effects of secondary combustion from heater hot surfaces was dependent on the combustion chamber air flow rate.

- Test running time. It took about 30 minutes to evacuate the animal test chamber. Another half hour or more was spent disassembling and cleaning the transfer line. General calibration and setup for the system was also substantially longer than for the cup furnace. Consequently, there was at least a doubling of the time required to conduct cone radiant heater tests compared to the NBS Toxicity Test Method.

With the NBS Toxicity Test Method, the  $LC_{50}$  (30 min and post-exposure) values were easily determined based on the amount of material loaded into the cup furnace or, when the residue was substantial, on the amount of material consumed. With the cone radiant heater toxicity test apparatus, difficulties, as noted above, were encountered in the determination of  $LC_{50}$  values. In some cases, insufficient combustion products were transferred to the animal exposure chamber. For example, even under conditions (i.e., low air flow rates, flux levels close to the materials' autoignition energy levels, maximum amounts of materials, etc.) designed to produce the maximum combustion products in the animal exposure chamber, no animal deaths were observed during or following exposures to either the flaming or non-flaming combustion products from either material tested singly. Therefore, the  $LC_{50}$  values could only be listed as greater than the highest concentrations attainable in the animal exposure chamber. However, when the composite, consisting of the fabric covered foam, was decomposed, some animal deaths occurred (Table 6) permitting  $LC_{50}$  values to be estimated as approximately 30 mg/l in the non-flaming mode and somewhere near 40 to 44 mg/l in the flaming mode. Lack of reproducibility prohibited statistical calculation of these values. These estimated  $LC_{50}$  values were not greatly different from those achieved with the cup (48 mg/l, non-flaming and

39 mg/l, flaming). These experimental results on the combined materials were also similar to those of the cup furnace in that post-exposure deaths occurred in the non-flaming mode and within-exposure deaths occurred in the flaming mode.

These experiments were also designed to determine if the combustion products generated from the single materials would be equivalent to those generated when the materials were combined. In both the flaming and non-flaming modes, the average concentration of the primary gases (CO, CO<sub>2</sub>, HCN) generated in the NBS Toxicity Test system from the thermal decomposition of the mixture of the materials appear to be approximately equal to (or, in the case of CO and HCN, slightly greater than) the sum of the average concentrations generated from the individual materials under the same conditions (Table 7). This means that if the concentrations of the primary gases that are generated from the thermal decomposition of the individual components are known, then a reasonable prediction of the gas concentrations from the mixture decomposed under the same conditions can be made. It is important to note that the respiration of the six animals in this closed system will produce an average gas concentration of approximately 2600 ppm of CO<sub>2</sub> in a 30 minute experiment. In the examination of the additivity of gas concentrations from the individual components, this respiration-generated CO<sub>2</sub> should only be considered once, since when the mixture is tested, there is only the contribution of one set of animals. This consideration is more important in the non-flaming mode since this amount of CO<sub>2</sub> represents a larger fraction of the combustion-generated CO<sub>2</sub> than that found in the flaming mode, which produces about 10 times more CO<sub>2</sub>.

Closer examination of these results, however, show that the average HCN levels from the flaming mixtures (Table 3) were higher than those seen in the flaming exposures of polyurethane alone at 525°C which, in turn, were greater than at 425°C (Table 1). This difference becomes more apparent when the HCN generation over time is examined rather than the average 30 minute concentrations.

Figure 11 shows the generation of HCN from 20 mg/l of the flexible polyurethane when decomposed alone or combined with the polyester under various flaming temperatures. The addition of various amounts of polyester to 20 mg/l of polyurethane at 525°C produced greater concentrations of HCN than in any of the experiments on the polyurethane alone (Tables 1, 3 and Fig. 11). This result was unexpected since polyester contains no nitrogen and should not contribute to the HCN generation. Figure 11 also shows that the HCN generation over time from 20 mg/l of flaming polyurethane foam alone tends to plateau during the 30 minute test, whereas, in the combination studies of this polyurethane (20 mg/l) and polyester, the HCN continues to increase throughout the experiments. The reason for this increased level of HCN is unexplained at this time.

In the flaming mode, the final concentrations of CO from the combined materials also appeared to be greater than the sum of the final CO concentrations from the individual materials (Fig. 12). This was more apparent from the graphic representation of the actual time generation of CO than from the tabular depiction of the average concentrations (Table 7). More experiments, however, are necessary to eliminate the possibility that this effect is due to experimental scatter. This apparent difference was not found in the non-flaming mode (Fig. 13).

The data obtained during this series of experiments also permitted the assessment of whether the animal deaths could be attributed to the concentrations of the primary toxic gases to which the animals were exposed. Recent results [15,16] from this laboratory on the toxicity of CO, CO<sub>2</sub> and HCN alone and in various combinations have shown that the 30 minute LC<sub>50</sub> for CO in air was 4600 ppm. No animals died below 4100 ppm or post-exposure. The 30 minute LC<sub>50</sub> for CO<sub>2</sub> in air was greater than 18% (1% = 10,000 ppm). However, when CO and CO<sub>2</sub> were combined, the presence of 5% CO<sub>2</sub> increased the toxicity of CO such that animals died from 30 minute exposures to CO concentrations of 2500 ppm. Some of these deaths occurred during the first 24 hours following the exposure. The combination of CO and HCN (30 minute HCN LC<sub>50</sub> = 160 ppm) showed the following additive effect:

$$\text{If } \frac{[\text{CO}]}{\text{LC}_{50} \text{ CO}} + \frac{[\text{HCN}]}{\text{LC}_{50} \text{ HCN}} \geq 1, \text{ the animals died.}$$

When this formula equalled less than 1, the animals lived. Again deaths were observed during the first 24 hours following the exposures.

Comparison of the CO, CO<sub>2</sub>, and HCN concentrations that were produced in the animal exposure chamber during the non-flaming and flaming polyurethane exposures with recent results from toxicity experiments on these gases alone and in various combinations [15] indicated less than lethal concentrations of these gases in all tests (Tables 1 & 4). For example, with the NBS system, at the highest loading of the polyurethane (40 mg/l), the average concentration of CO during a non-flaming experiment was 740 ppm, CO<sub>2</sub> was 2500 ppm, and HCN was below detectable limits. In a flaming experiment at 40 mg/l, the CO was

840 ppm, CO<sub>2</sub> was approximately 33500 ppm, and HCN was 27 ppm. All of these gases, even if considered in combination, were not sufficient to cause lethality at these concentrations. Therefore, the post-exposure deaths from polyurethane seen in the non-flaming mode in the NBS system were due to one or more toxic combustion products or some other undetermined factors that were not measured in these experiments. These deaths were noted as late as 14 days following exposure.

Examination and comparison of the average gas concentrations that were generated during the lethal NBS Toxicity Test Method non-flaming polyester experiments with our pure gas toxicity experiments indicate that the average CO levels were 56-63% of that necessary to cause death by CO alone (4600 ppm) [15]. The maximum CO levels in the lethal experiments were 78-89% of the lethal CO concentration. The average CO<sub>2</sub> present was about 10% of that necessary to increase the susceptibility of the rats to lower levels of CO (e.g., 50,000 ppm of CO<sub>2</sub> caused rats to die at approximately 2500 ppm of CO [16]). The COHb levels at the end of the 30 minute lethal exposures were 75-83%. In a separate series of experiments in which the animals were exposed to pure CO in air for 30 minutes, no deaths were observed in animals with COHb levels below 83%. These results indicate that CO was contributing to the within-exposure deaths, but that other toxic or irritant gas(es) or undetermined factors were also acting in conjunction with or to potentiate the effects of the CO. The cause of the late post-exposure deaths is also unexplained.

Non-flaming experiments on the polyester in the NBS system at a lower temperature (375°C) produced no deaths even at concentrations as high as 50 mg/l. The gas data were in agreement with these results.

Examination of the gases generated during the lethal experiments from different mass loadings of polyester decomposed by the NBS Toxicity Test Method in the flaming mode shows that the average CO varied between 2300-3000 ppm and the CO<sub>2</sub> varied between 2.7% - 3% (1% = 10,000 ppm). In these lethal experiments, the COHb levels ranged from 83-85% and the rats died within exposure or shortly thereafter. These COHb results would implicate CO or CO plus CO<sub>2</sub> as the main toxicants. However, the average CO was approximately 50-65% of the lethal concentration determined for CO alone. Even considering the synergistic effect of CO<sub>2</sub> on CO, the average values of CO and CO<sub>2</sub> from flaming polyester were still too low to account for the deaths that occurred during these 30 minute exposures. Only if one considered the maximum CO levels along with the CO<sub>2</sub> concentrations would the deaths be predictable.

When the polyester was decomposed in the flaming or non-flaming mode with the cone radiant heater apparatus, there was not enough CO and/or CO<sub>2</sub> transferred to the animal exposure chamber to cause any deaths.

The NBS Toxicity Test Method experiments on the combined polyurethane and the polyester indicated that both materials contributed to the resultant toxicity. In the non-flaming mode at 375°C, 20 mg/l of the polyester (a non-lethal concentration at this temperature) increased the toxicity of the combined materials 10 mg/l over that expected if the polyester were truly non-toxic as

indicated when tested alone at this temperature. All deaths occurred during the post-exposure period in a similar manner to that observed with the polyurethane by itself. The concentrations of measured gases (CO, CO<sub>2</sub>, HCN) that were generated during these exposures were not sufficient even in combination to have produced any within-exposure deaths. These measured gases were also not responsible for the post-exposure deaths that occurred.

Some post-exposure deaths were observed in the non-flaming combination experiments conducted with the radiant cone heater. In these combined experiments, the gases transferred to the animal exposure chamber were not sufficient to have produced within-exposure deaths and no such deaths were observed.

When the combined materials were tested by the NBS Toxicity Test Method in the flaming mode at 525°C, both materials contributed in an additive fashion to the combined toxicity. The LC<sub>50</sub> (30 min and 14 day) value of 39 mg/l resulted from the addition of 20 mg/l of the polyurethane to 19 mg/l of polyester, although concentrations (ranging from 20-40 mg/l) of flaming combustion products from the polyurethane alone caused no deaths. In other words, a non-lethal amount of the polyurethane (20 mg/l) plus a non-lethal amount of the polyester (20 mg/l) caused 50% of the animals to die within the 30 minute exposure. Examination of the average gas concentrations of CO, CO<sub>2</sub>, and HCN which were generated during these flaming exposures and comparison of these gas values with our pure gas toxicological studies shows that the concentrations of these gases were sufficient to account for the deaths that occurred.

In the flaming combined radiant cone heater experiments, the levels of CO, CO<sub>2</sub>, and HCN were also sufficient to account for the within-exposure deaths that occurred.

## 5. CONCLUSIONS

A flexible polyurethane foam and a polyester fabric, two common components of commercially available upholstered chairs were examined with the NBS Toxicity Test Method and with a cone radiant heater toxicity apparatus. In both cases, the fabric and foam were heated individually and then together.

The NBS Toxicity Test experiments indicated that for the individual materials:

- The decomposition products of the flexible polyurethane foam produced no deaths during exposure and only caused post-exposure deaths in the non-flaming mode.
- The polyester when decomposed 25°C above or below its autoignition temperature caused deaths both during and following exposures.

Comparison of the CO, CO<sub>2</sub>, and HCN concentrations generated from the individual materials with pure gas toxicity experiments (performed with single and multiple gases) indicated:

- The deaths from flexible polyurethane could not be explained by the concentrations of these gases.

- Non-flaming polyester produced relatively high COHb (75-83%) levels, but lower than lethal average or maximum CO concentrations. Even when CO was considered with CO<sub>2</sub> (which acts synergistically with CO), the combination was not sufficient to account for the deaths.
- The deaths from exposures to flaming polyester products were probably due to CO since COHb values were 83-85%. In this case, the maximum (not the average) concentrations of CO plus CO<sub>2</sub> were sufficient to predict the deaths.

Results of combusting combined materials in the NBS Toxicity Test Method indicated that:

- Depending on the amount thermally decomposed, both materials contributed to the combined toxicity. In the flaming mode, the contribution was additive.
- Similar to the polyurethane results, the non-flaming combined experiments produced only post-exposure deaths and these could not be explained by the generated CO, CO<sub>2</sub>, and HCN concentrations.
- The deaths observed from the flaming combined experiments were explainable based on the concentrations of CO, CO<sub>2</sub>, and HCN.

Comparison of the gas concentrations from the combined materials with those from the individual materials indicated:

- The non-flaming yields of CO, CO<sub>2</sub>, and HCN appear to be approximately equal to the sum of the yields from the single materials.
- The flaming yields of HCN were greater than the sum of those from the single materials.

The cone radiant heater toxicity test apparatus, as currently designed, did not provide good reproducible results. LC<sub>50</sub> values could only be roughly estimated for the combined material experiments; these values (approximately 30 mg/l in the non-flaming mode and somewhere near 40 to 44 mg/l in the flaming mode) were not greatly different from those achieved with the cup furnace (48 mg/l in the non-flaming mode and 39 mg/l in the flaming mode). The results that were obtained showed that the concentrations of the primary gases in the exposure chamber could be used to predict whether deaths would occur. In the experiments on the combined materials, the cone radiant heater results were similar to those of the cup furnace in that post-exposure deaths occurred in the non-flaming mode and within-exposure deaths occurred in the flaming mode.

The results of this study have shown that satisfactory toxicity screening results on composite materials can be achieved with the use of the NBS Toxicity Test Method. Composites for which it is known that the surface materials do not offer a substantial fire barrier protection to the underneath layers can be

tested simply as an agglomeration, instead of a layered composite. (At the other extreme, interstitial materials which are very adequately protected from fire involvement by the surface layer may not need to be tested at all.) There is an intermediate regime, where the surface layers act to slow down, but not to wholly eliminate, the burning of the underneath layers. If a detailed characterization of such construction is required, it is possible, in principle, to determine in the Cone Calorimeter the relative involvement of the layers, and then to conduct several NBS toxicity tests using individual materials or combinations.

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Table 1

## Toxicity Results for Flexible Polyurethane #13 Using the NBS Toxicity Test Method

Material	AIT (°C)	Mode	Initial Temp. of Expt. (°C)	Type of Expt.	Mass Chamber Vol.		Average Gas Concentration <sup>1</sup>			Max. CO (ppm)	Highest % COHb (30 min)	No. tested Within Exp. & Post Death	Latest Day of Death	LC <sub>50</sub> 30 min. + 14 days (mg/l)
					Loaded (mg/l)	Consumed (mg/l)	CO (ppm)	CO <sub>2</sub> (ppm)	O <sub>2</sub> (%)					
Poly- urethane #13	400	NF	374	A	10.0	9.3	420	470	20.8	8	540	NA	NA	
			375	R	19.8	17.9	620	2370	20.4	ND	800	0/6	14	
			375	R	30.0	26.6	700	2690	20.4	4	1000	0/6	11	37.0
			375	R	32.0	27.4	600	2800	20.3	5	1100	0/6	7	(29.8-46.0)*
			377	R	35.0	31.1	ND	ND	ND	9	ND	0/6	11	
		375	R	40.0	34.3	740	2500	ND	1	1320	0/6	12		
Poly- urethane #13	400	F	425	A	10.0	9.7	170	8700	19.9	19	210	NA	NA	
			425	R	20.0	19.9	320	21400	18.2	17	370	0/6	NA	>40
			425	R	30.0	29.8	520	28400	17.4	24	590	0/6	NA	
			425	R	40.0	39.1	840	33500	16.7	27	940	0/6	NA	
			524	A	20.0	19.9	630	10700	19.5	51	720	NA	NA	
		528	A	20.0	19.9	390	19100	18.7	37	430	NA	NA		

Legend:

1. Average gas concentration =  $\frac{\text{integrated area under instrument response curve for 30 minutes}}{30 \text{ minutes}} = \text{ppm-min}$

A. Analytical experiment

R. Rat experiment

ND. Not determined

NA. Not applicable

F. Flaming

NF. Non-flaming

AIT. Auto-ignition temperature

\*, 95% confidence limits

FPU 13. Flexible polyurethane #13

PE. Polyester

Comb. Combined weight of FPU 13 + PE

Table 2  
Toxicity Results for the Polyester Fabric Using the NBS Toxicity Test Method

Material	AIT (°C)	Mode	Initial Temp. of Expt. (°C)	Type of Expt.	Mass Chamber Vol.		Average Gas Concentration <sup>1</sup>			Max. CO (ppm)	HCN (ppm)	O <sub>2</sub> (%)	Highest % COHb (30 min)	No. died		Latest Day of Death	LC <sub>50</sub> 30 min. + 14 days (mg/ℓ)			
					Loaded (mg/ℓ)	Consumed (mg/ℓ)	CO (ppm)	CO <sub>2</sub> (ppm)	Within Exp.					Within & Post						
Polyester	500	NF	474	A	20.0	16.4	970	1700	20.7	NA	1270	NA	NA	NA	NA	NA	NA			
			474	A	25.0	21.3	1670	2550	20.6	NA	2330	NA	NA	NA	NA	NA	NA	NA		
			473	R	35.0	30.6	2440	4770	20.5	NA	3460	81.6	0/6	0/4	NA	NA	NA	NA		
			473	R	36.5	30.9	2330	4910	20.4	NA	3140	67.8	0/6	0/4	NA	NA	NA	NA		
			476	R	37.1	32.5	2810	5590	20.3	NA	3900	83.7	0/6	0/4	NA	NA	NA	NA	39.0	
			475	R	37.5	32.4	2570	5350	20.4	NA	3590	79.3	1/6	5/5	2	2	2	2	(38.4-39.5)*	
			475	R	38.5	34.3	2910	5920	20.3	NA	4090	82.7	2/6	3/6	2	2	2	2		
			473	R	39.2	33.2	2650	5300	20.4	NA	3730	75.0	2/6	3/5	2	2	2	2		
			475	R	40.0	34.9	2660	4990	20.4	NA	3830	81.0	4/6	5/6	1	1	1	1		
			377	A	20.0	4.3	50	600	20.9	NA	160	NA	NA	NA	NA	NA	NA	NA	NA	
			376	R	40.0	21.9	370	2980	20.5	NA	770	13.5	0/6	0/4	NA	NA	NA	NA	>50	
			375	R	50.0	20.4	410	2710	20.6	NA	840	15.2	0/6	0/5	NA	NA	NA	NA		
Polyester	500	F	524	R	30.0	28.7	2220	25200	18.4	NA	2990	82.0	0/6	0/4	NA	NA	37.5			
			525	R	35.0	33.7	2290	27300	18.2	NA	3400	83.0	1/6	2/5	0	0	0	(35.3-39.8)*		
			523	R	37.5	36.1	2640	28500	18.0	NA	3860	83.2	3/6	3/6	NA	NA	NA			
			524	R	40.0	38.8	2990	30500	17.8	NA	4310	84.6	4/6	4/5	NA	NA	NA			

For Legend, see Table 1

Table 3

## Toxicity Results for Flexible Polyurethane #13 Plus Polyester Using the NBS Toxicity Test Method

Material (°C)	AIT Mode (°C)	Initial Type Temp. of Expt. Expt. (°C)	Mass/Chamber Volume			Consumed (mg/l)	Average Gas Concentration <sup>1</sup>			Max. CO (ppm)	Highest % COHb (30 min)	No. died		Latest Day of Death	LC <sub>50</sub> 30 min. + 14 days (mg/l)		
			FPU 13	PE	Comb.		CO (ppm)	O <sub>2</sub> (%)	HCN (ppm)			Within Exp.	Post				
Polyester plus poly- urethane #13	500	NF	373	R	20.0	20.0	40.0	21.0	690	2600	20.5	ND	890	31.9	0/6	0/4	NA
			375	R	27.5	20.0	47.5	26.2	670	3120	20.5	ND	960	26.4	0/6	2/4	8
			373	R	30.0	20.0	50.0	31.2	850	3400	20.5	5	1270	35.2	0/6	3/4	7
			373	R	32.5	20.0	52.5	33.4	1130	3920	20.3	ND	1420	43.9	0/6	3/4	2
			374	R	35.0	20.0	55.0	35.4	1300	3810	20.4	ND	1710	35.4	0/6	4/4	16
		376	R	37.5	20.0	57.5	37.3	1390	3850	20.4	ND	1860	54.9	0/6	4/4	2	
		375	R	40.0	20.0	60.0	43.1	1160	4090	20.4	ND	1550	40.9	0/6	4/4	2	
		376	R	29.9	47.5	77.4	47.9	880	3510	20.5	ND	24.3	24.0	0/6	3/5	9	
		375	R	34.8	47.5	82.3	46.7	380	2620	20.6	ND	24.3	ND	0/6	1/5	1	
Polyester plus poly- urethane #13	500	F	527	R	20.0	15.0	35.0	34.0	1870	30200	17.5	62	2370	76.2	1/6	1/5	NA
			523	R	20.0	20.0	40.0	38.9	2270	33600	17.1	63	3120	80.2	3/6	3/5	NA
			525	R	20.0	22.5	42.5	41.8	2410	31100	17.4	50	3420	78.7	5/6	5/6	NA
			524	R	20.0	25.0	45.0	44.0	2780	34400	16.8	48	3930	ND	6/6	6/6	NA
			524	R	20.0	30.0	50.0	49.0	3070	34700	17.1	59	4500	ND	6/6	6/6	NA
		425	R	20.0	30.0	50.0	43.7	1750	31500	17.4	13	1950	69.1	1/6	1/5	NA	

For legend, see Table 1

TABLE 4

## Toxicity Results for Flexible Polyurethane #13 Using the Cone Radiant Heater

Mode	Combustion Chamber Conditions			Exposure Chamber Conditions					Animal Results				
	Expt. flux <sup>b</sup> (W/cm <sup>2</sup> )	Air flow (L/min)	Mass loaded (g)	Mass consumed (g)	Gas Sampling Time Initial (min:sec)	Gas Sampling Time End (min:sec)	CO Init./final (ppm)	CO <sub>2</sub> Init./final (ppm)	O <sub>2</sub> Avg. (%)	HCN Avg. (ppm)	Conc <sup>a</sup> (mg/L)	# died/# tested	Within Exposure
NF	2.0	25	13.0	7.0	4:00	11:00	630/630	1700/4870	20.6	ND	22	0/6	0/6
		25	14.0	6.3	4:00	11:15	500/440	1600/5680	20.5	ND	19	0/6	0/6
		15	12.8	5.3	5:00	14:50	520/470	1670/5340	20.6	6	15	0/6	0/6
F		5	11.9	11.8	5:00	18:40	470/390	970/3130	20.9	6	29	0/6	0/6
	2.0	60	13.3	7.5	1:00	5:40	1120/1040	36700/41380	16.1	ND	14	0/6	0/6
		40	13.1	ND	2:00	7:40	1690/1583	42080/44870	15.6	ND	-	0/6	0/6
		25	13.9	7.9	2:00	10:10	11400/1010	41000/44840	15.7	20	21	0/6	0/6

a. See Appendix A

b. Flux at which experiments were conducted. Flaming was initiated by an electrical spark. Autoignition flux was 2.08 W/cm<sup>2</sup>.

ND. Not determined

NF. Non-flaming

F. Flaming

TABLE 5

## Toxicity Results for the Polyester Fabric Using the Cone Radiant Heater

Mode	Combustion Chamber Conditions			Exposure Chamber Conditions					Animal Results		
	Expt. flux <sup>b</sup> (W/cm <sup>2</sup> )	Air flow (l/min)	Mass loaded (g)	Gas Sampling Time Initial (min:sec)	Gas Sampling Time End (min:sec)	CO Init./final (ppm)	CO <sub>2</sub> Init./final (ppm)	O <sub>2</sub> Avg. (%)	HCN Avg. (ppm)	Conca (mg/l)	# died/# tested
NF	2.0	25	23.9	2:00	8:00	100/100	650/650	20.9	ND	<5	NAC
F	3.5	25	23.8	2:00	12:00	1900/1840	49780/53740	15.9	ND	41	0/6

- a. See Appendix A  
 b. flux at which experiments were conducted. Flaming was initiated by an electrical spark. Autoignition flux was 4.0 W/cm<sup>2</sup>.  
 c. no animals were exposed in this experiment due to low concentrations of combustion products.  
 ND. not determined  
 NF. non-flaming  
 F. flaming

TABLE 6

## Toxicity Results for Flexible Polyurethane #13 plus Polyester Using the Cone Radiant Heater

Mode	Combustion Chamber Conditions			Exposure Chamber Conditions					Animal Results			
	Expt. flux <sup>b</sup> (W/cm <sup>2</sup> )	Air flow (l/min)	Mass loaded (g)	Gas Sampling Time Initial (min:sec)	Time End (min:sec)	CO Init./final (ppm)	CO <sub>2</sub> Init./final (ppm)	O <sub>2</sub> Avg. (%)	HCN Avg. (ppm)	Conc <sup>a</sup> (mg/l)	# died/# tested	Within plus post
NF	2.0	15	23.7	5:00	14:20	580/470	1290/3160	20.7	ND	22	0/6	0/6
		25	24.0	5:00	12:15	790/600	800/3290	20.7	ND	31	0/6	3/6 <sup>c</sup>
F	2.0	25	25.5	2:00	10:10	2130/1980	51840/53740	15.8 <sup>e</sup>	22	40	0/6	0/6
		25	24.7	2:00	9:20	3650/3420	55600/55950	16.4 <sup>d</sup>	28	44	5/6	5/6

a. See Appendix A

b. flux at which experiments were conducted. Flaming was initiated by an electrical spark.

c. 2/6 animals died within 14 days; one died on day 25.

d. O<sub>2</sub> added to exposure chamber.

e. O<sub>2</sub> added to exposure chamber which was then backfilled with air.

ND. not determined

NF. non-flaming

F. flaming

Table 7

Gas Concentrations from the Thermal decomposition of  
Polyurethane Foam and Polyester Alone and in Combination  
by the NBS Toxicity Test Method

Mode	Temp. (°C)	Material	Mass Loaded Chamber Volume (mg/ℓ)	Average Gas Concentration <sup>1</sup>		
				CO (ppm)	CO <sub>2</sub> (ppm)	HCN (ppm)
Flaming	525	Polyurethane	20 <sup>2</sup>	510 (+ 120)	14900 (+ 4200)	44 (+ 7)
		Polyester	30	<u>2220</u>	<u>25200</u>	--
		Total		2730	40100	44
		Polyurethane + Polyester	20 + 30	3070	34700	59
Non- Flaming	375	Polyurethane	30	700	2690	4
		Polyester	20 <sup>3</sup>	<u>50</u>	<u>600</u>	--
		Total		750	3290	4
		Polyurethane + Polyester	20 + 30	850	3400	5

1 Average gas concentration:

$$\frac{\text{integrated area under instrument response curve for 30 minutes}}{30 \text{ minutes}} = \frac{\text{ppm-min}}{30 \text{ min}}$$

2 Results are average ± range of two analytical experiments

3 Analytical experiment (no animals)

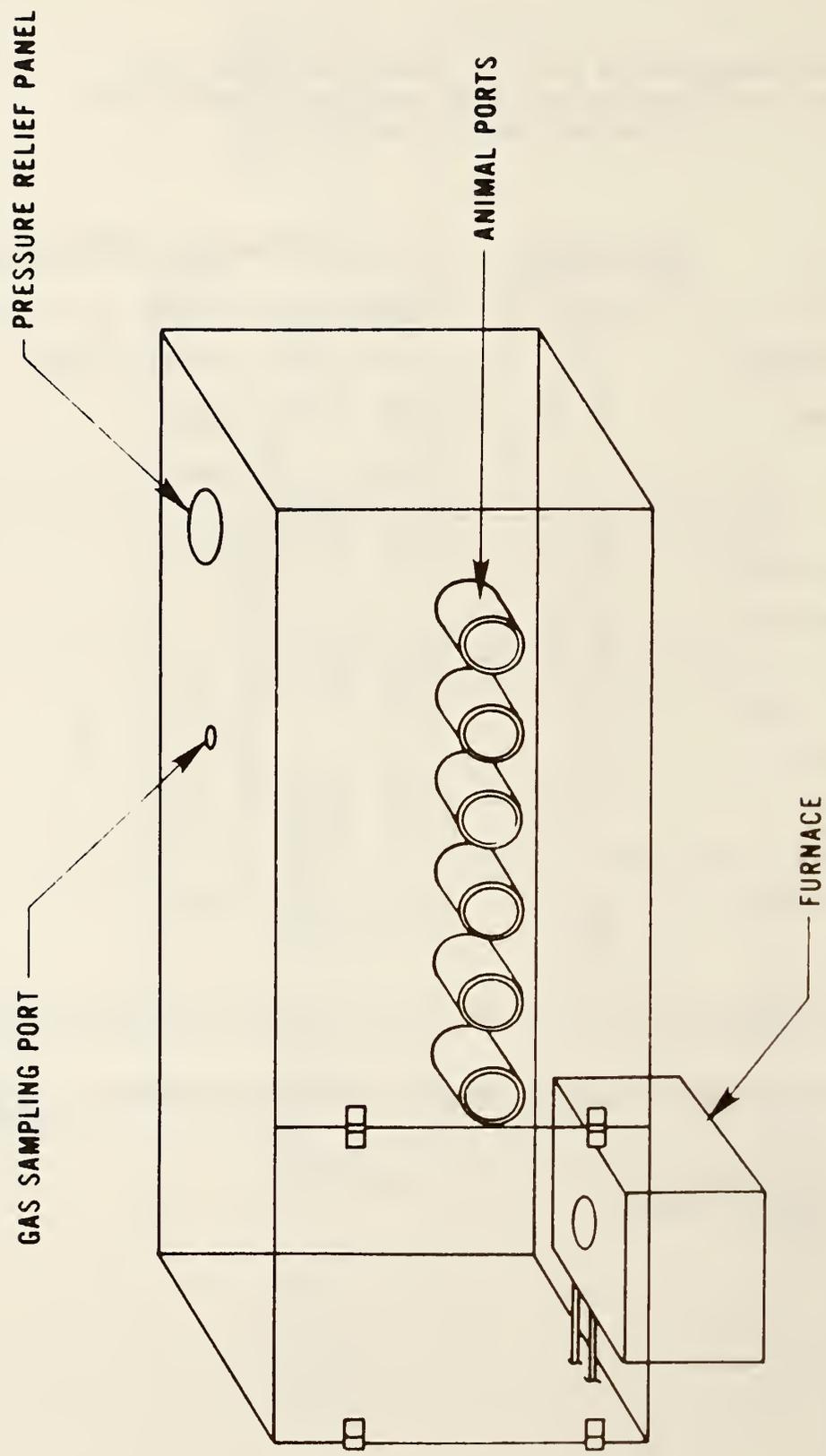


Figure 1. NBS Toxicity Test Method animal exposure chamber and furnace

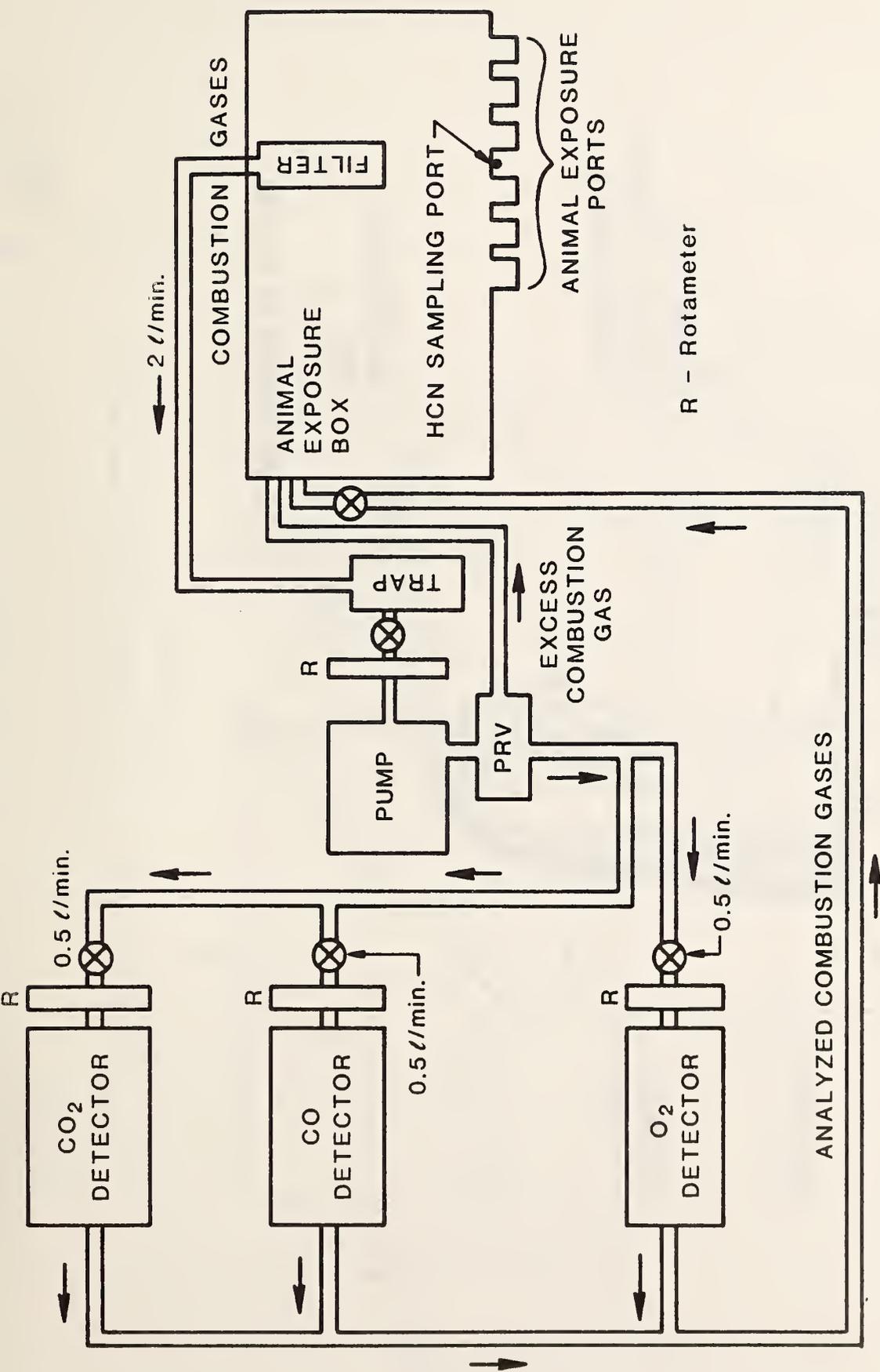


Figure 2. Schematic of NBS Toxicity Test Method and gas analysis system

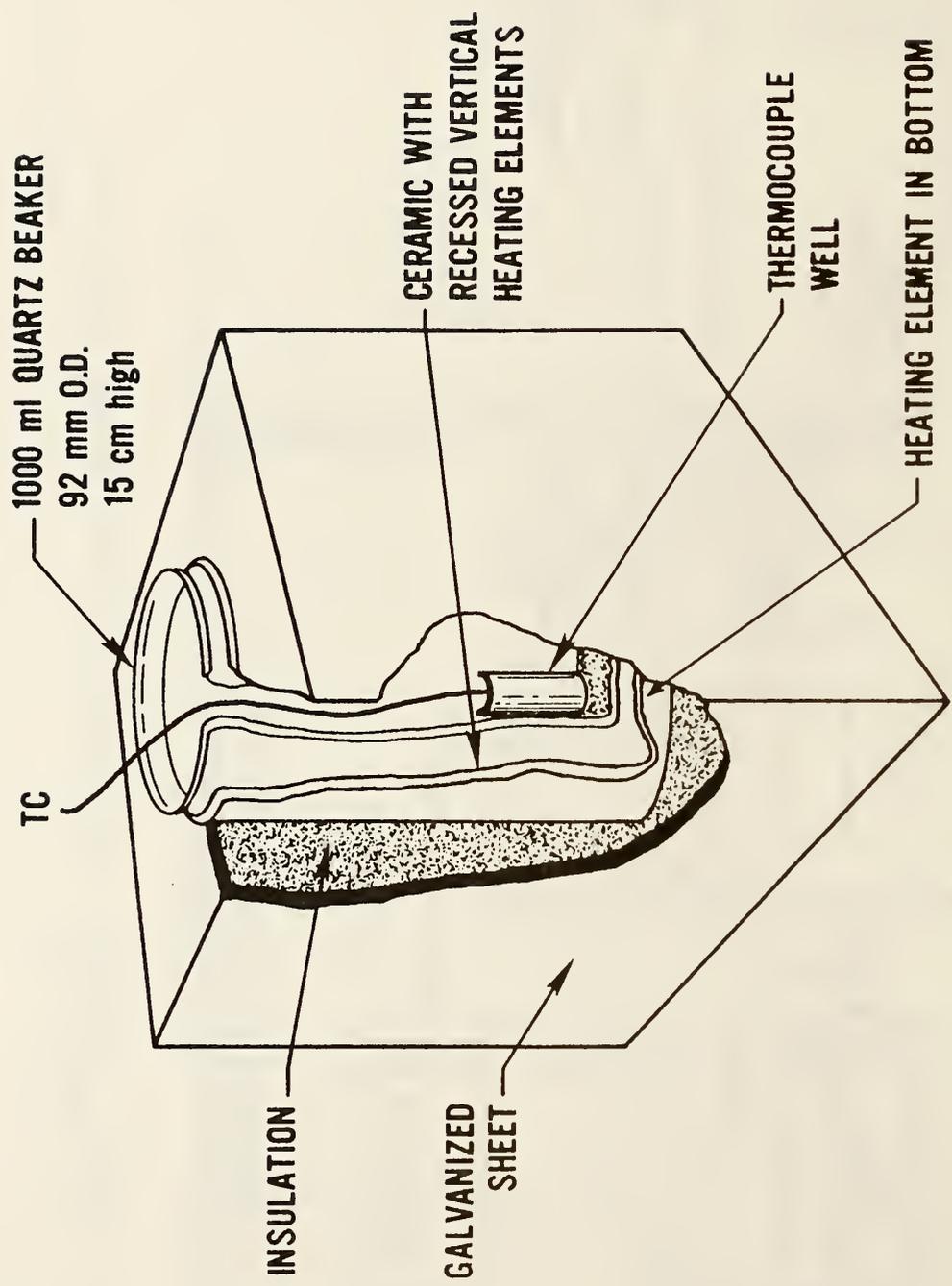


Figure 3. NBS Toxicity Test Method pyrolysis/combustion furnace

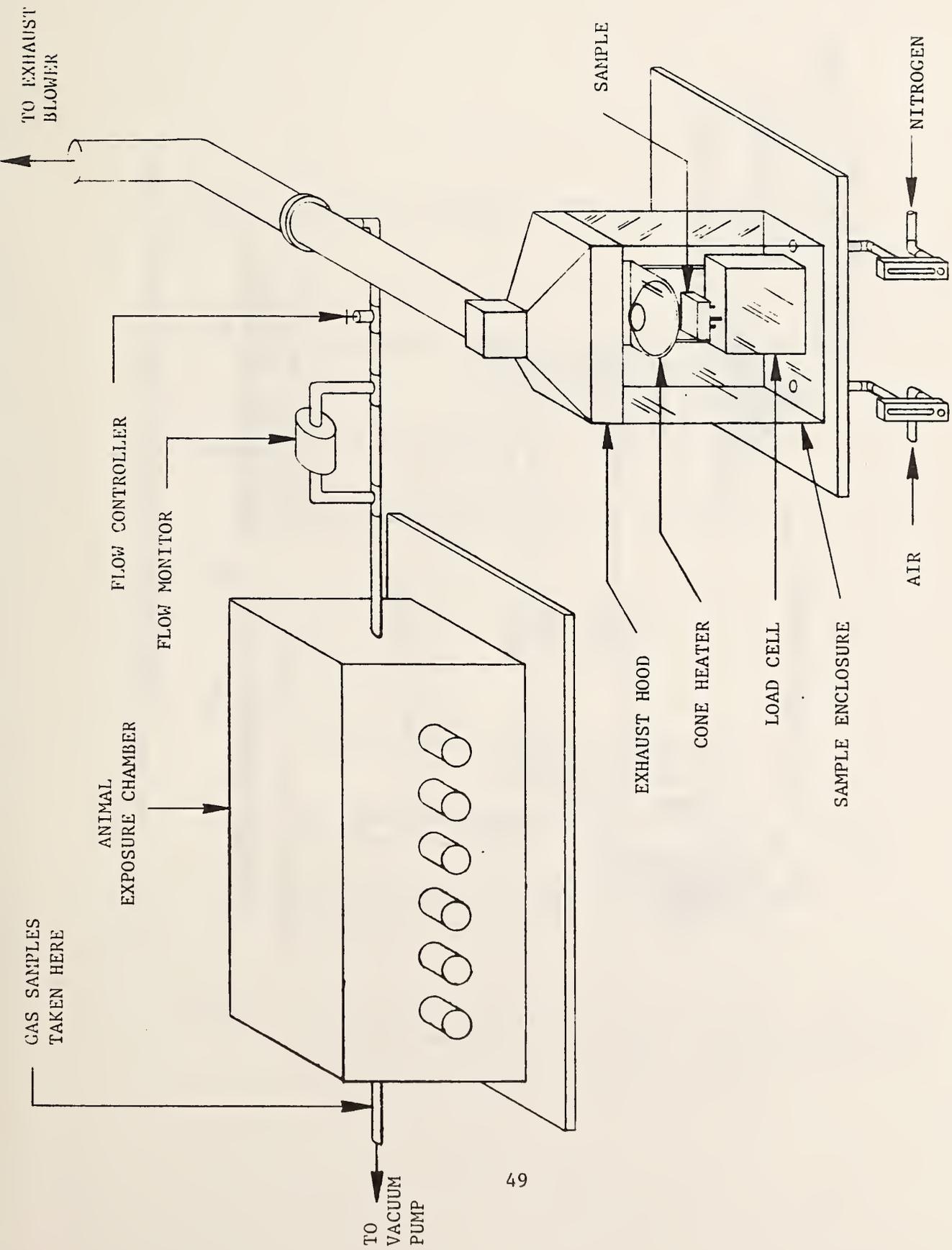


Figure 4. Cone radiant heater toxicity test apparatus

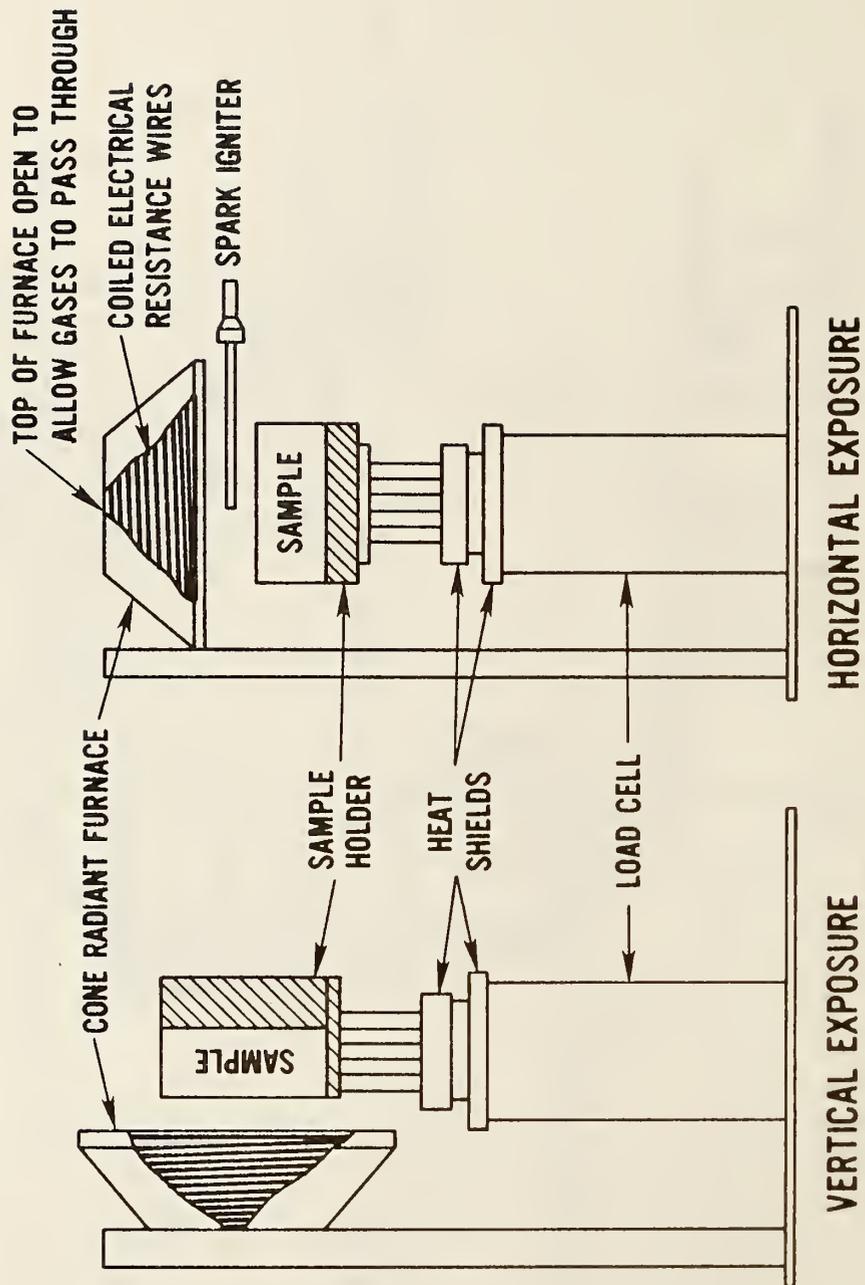


Figure 5. The cone radiant furnace in vertical and horizontal modes

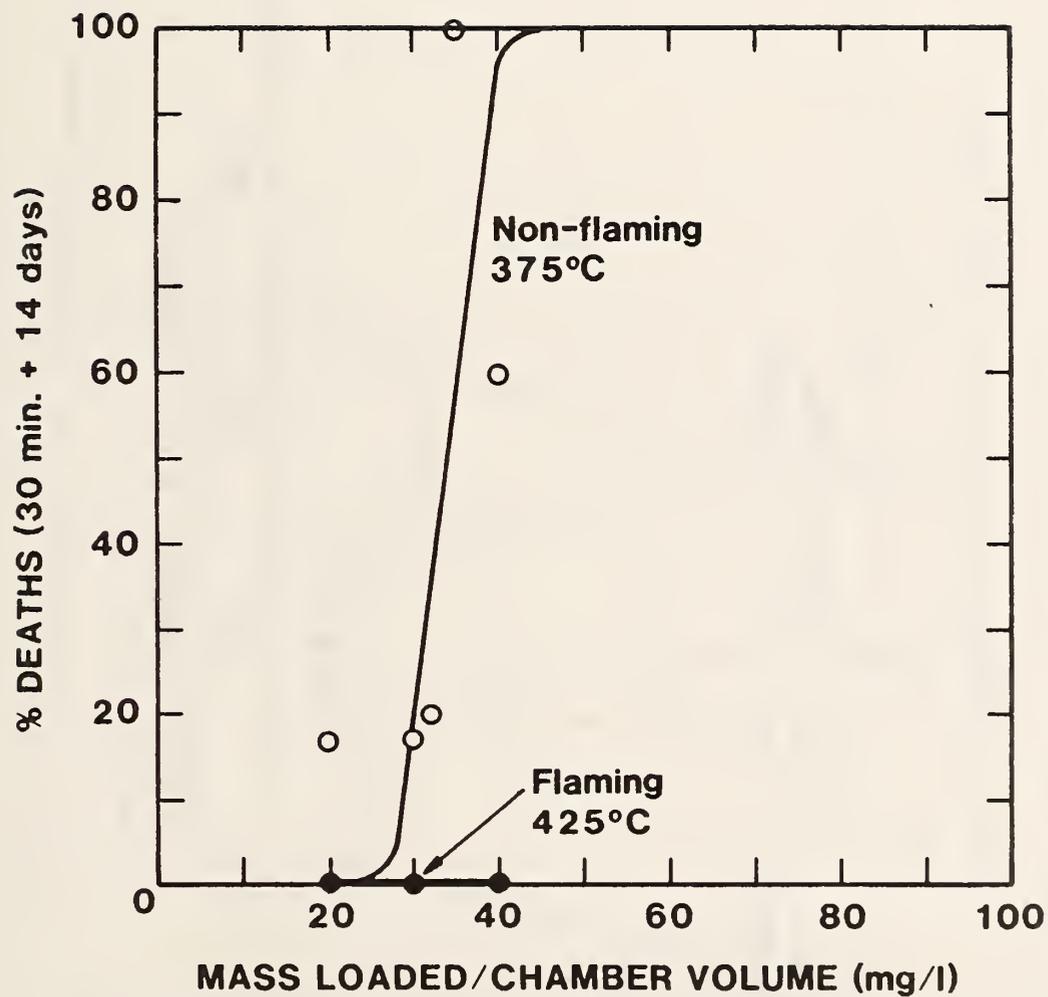


Figure 6. Concentration-response curves for flexible polyurethane foam (NBS Toxicity Test Method). All deaths occurred during the 14 day post-exposure period

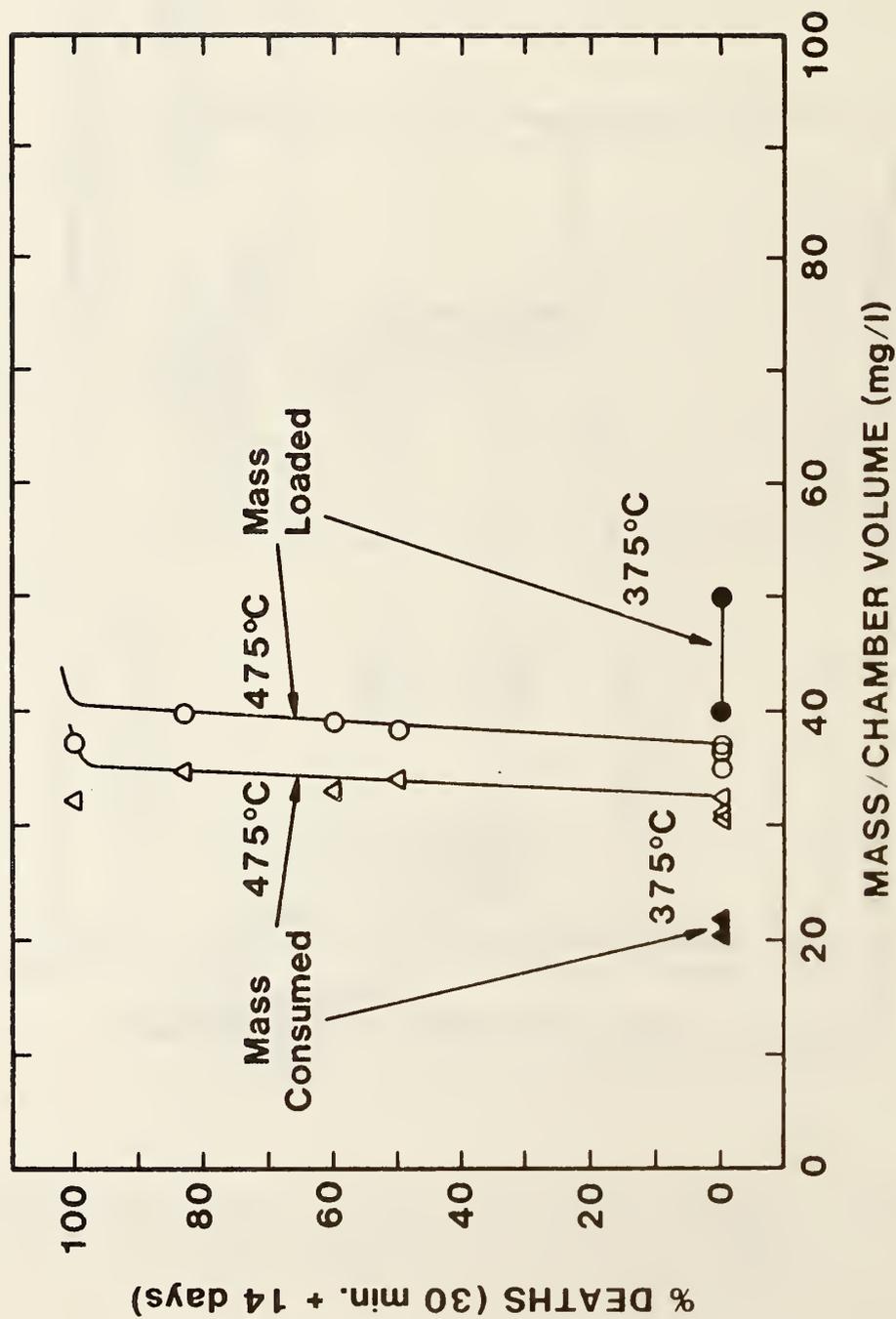


Figure 7. Concentration-response curves for polyester decomposed in the non-flaming mode (NBS Toxicity Test Method)

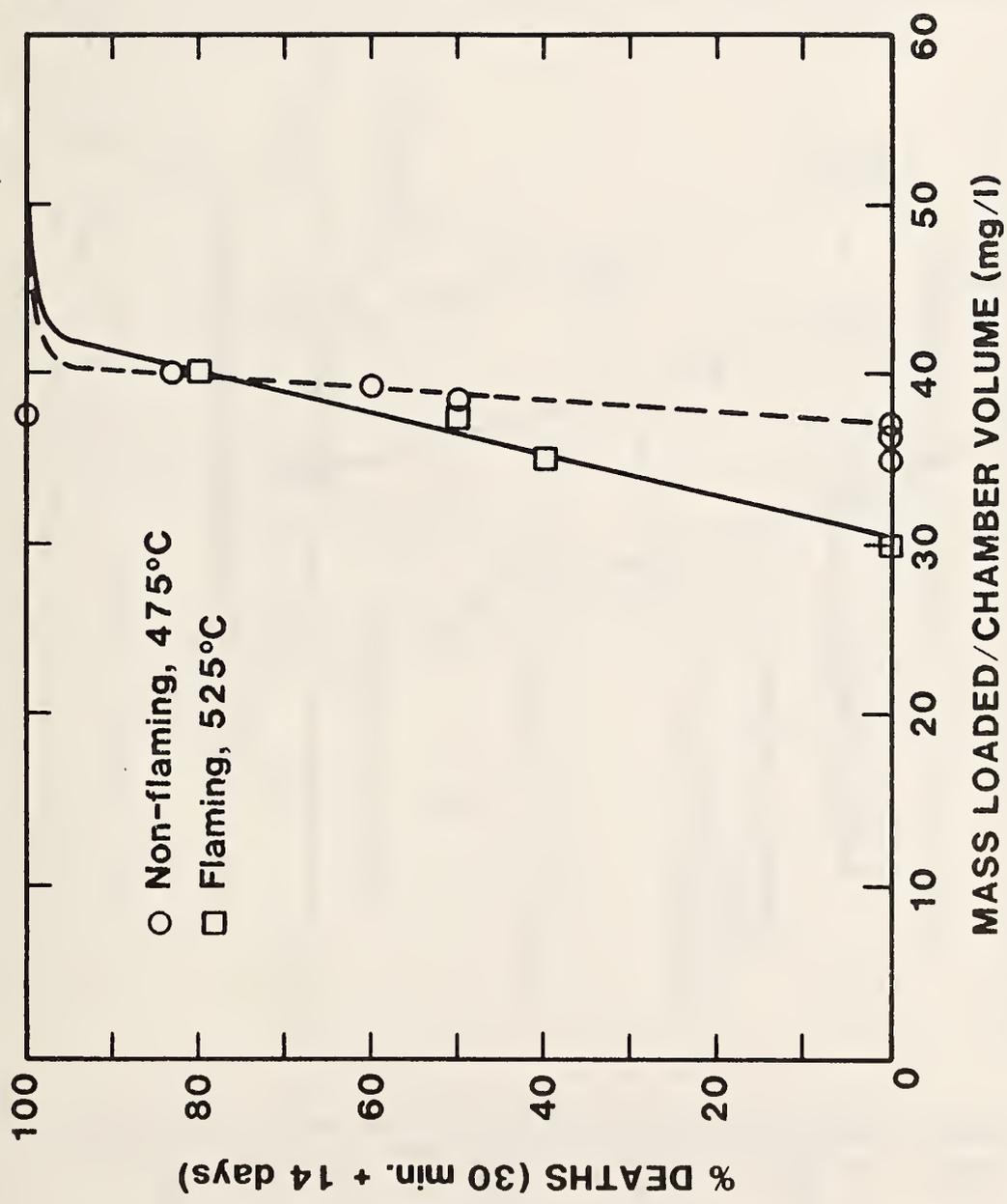


Figure 8. Concentration-response curves for polyester decomposed 25°C above and below its autoignition temperature (NBS Toxicity Test Method)

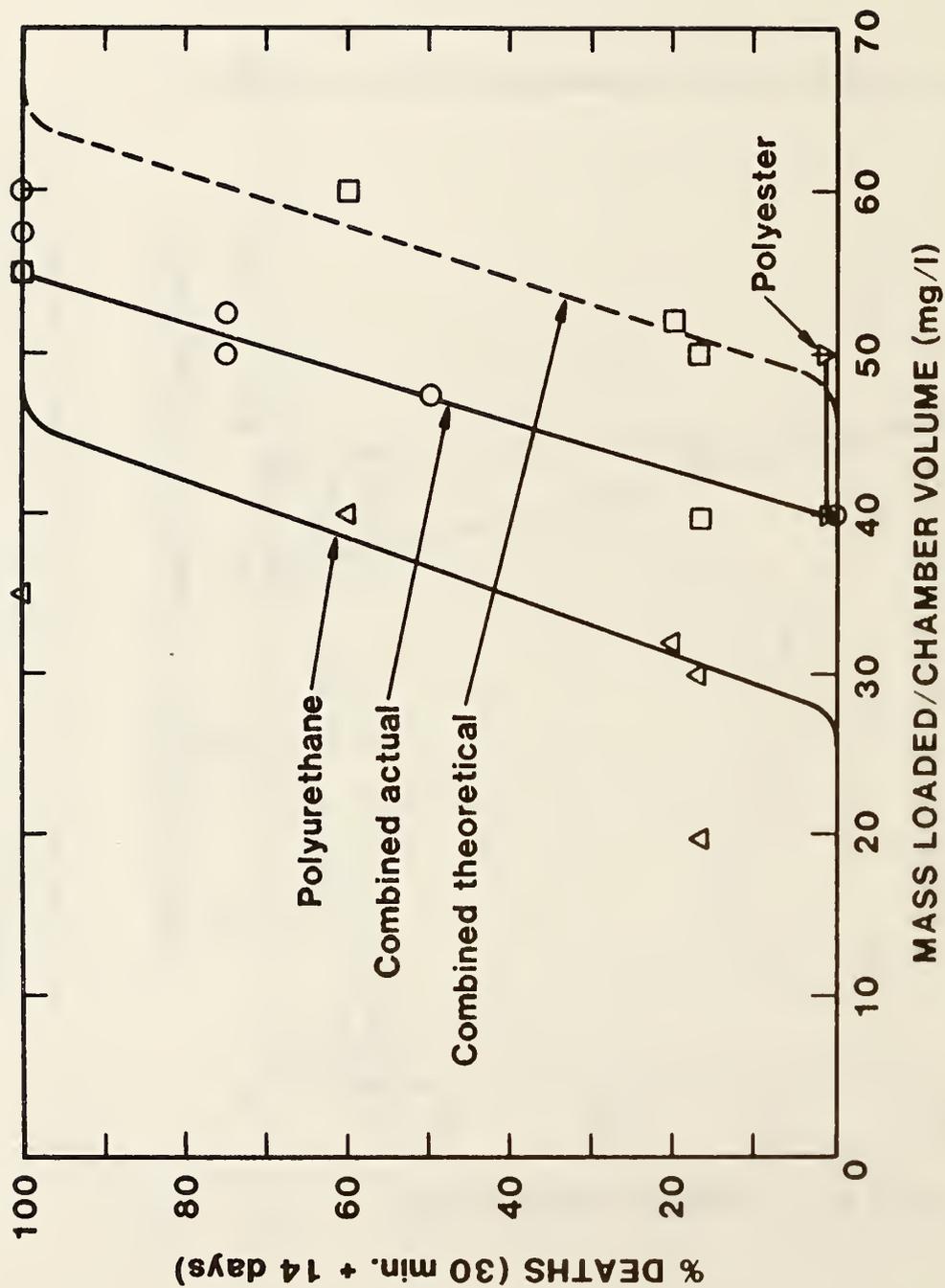


Figure 9. Concentration-response curves for polyurethane alone, polyester alone, and a mixture of polyurethane and polyester (20 mg/l), all of which were decomposed in the non-flaming mode at 375°C (NBS Toxicity Test Method). Also shown is the combined theoretical concentration-response curve based on the polyurethane plus the addition of 20 mg/l of an inert material

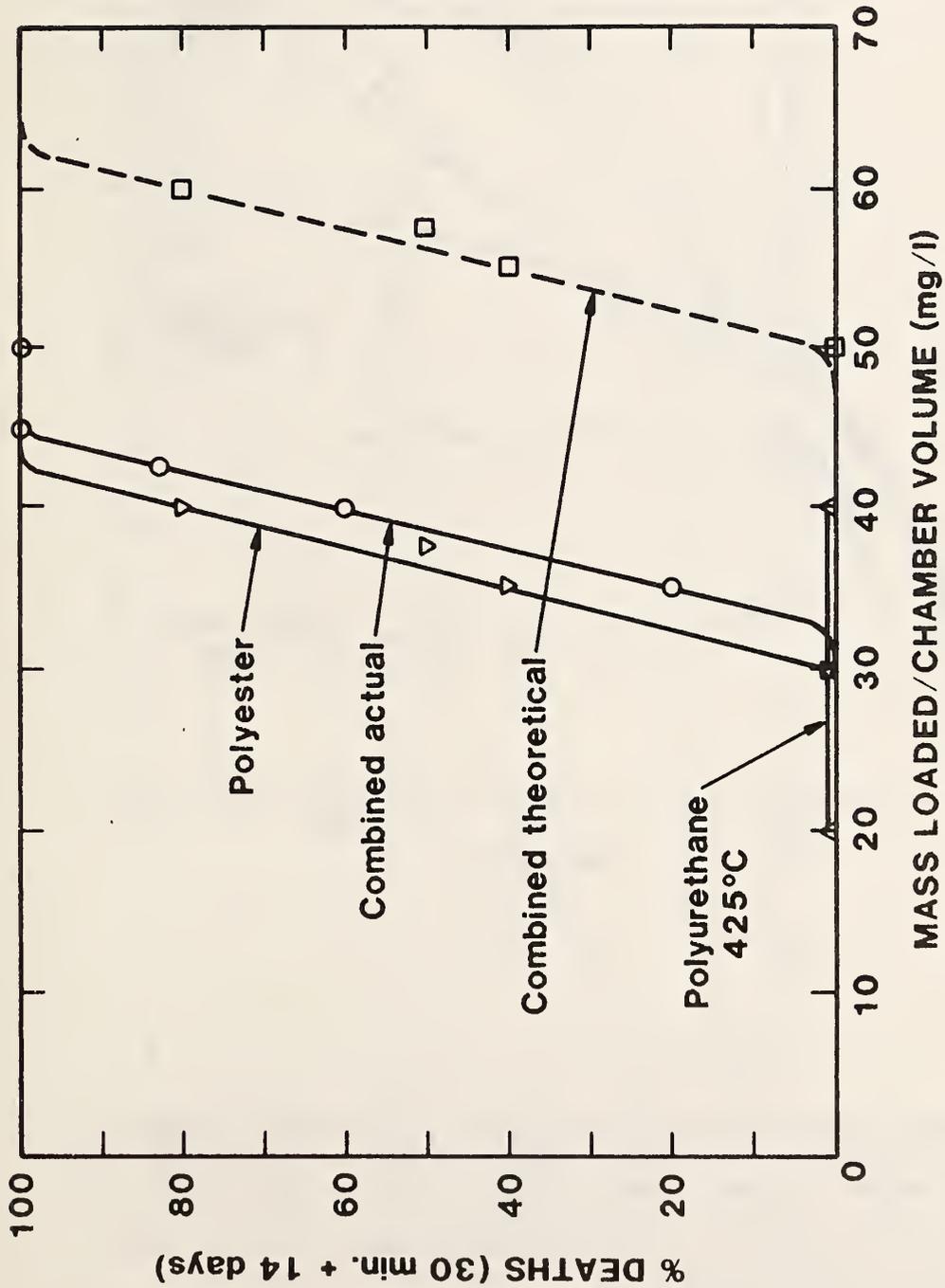


Figure 10. Concentration-response curves for polyester alone (flaming, 525°C) polyurethane alone (flaming 425°C) and polyester plus polyurethane (20 mg/l) decomposed in the flaming mode at 525°C (NBS Toxicity Test Method). Also shown is the combined theoretical concentration-response curve based on polyester plus 20 mg/l of an inert material.

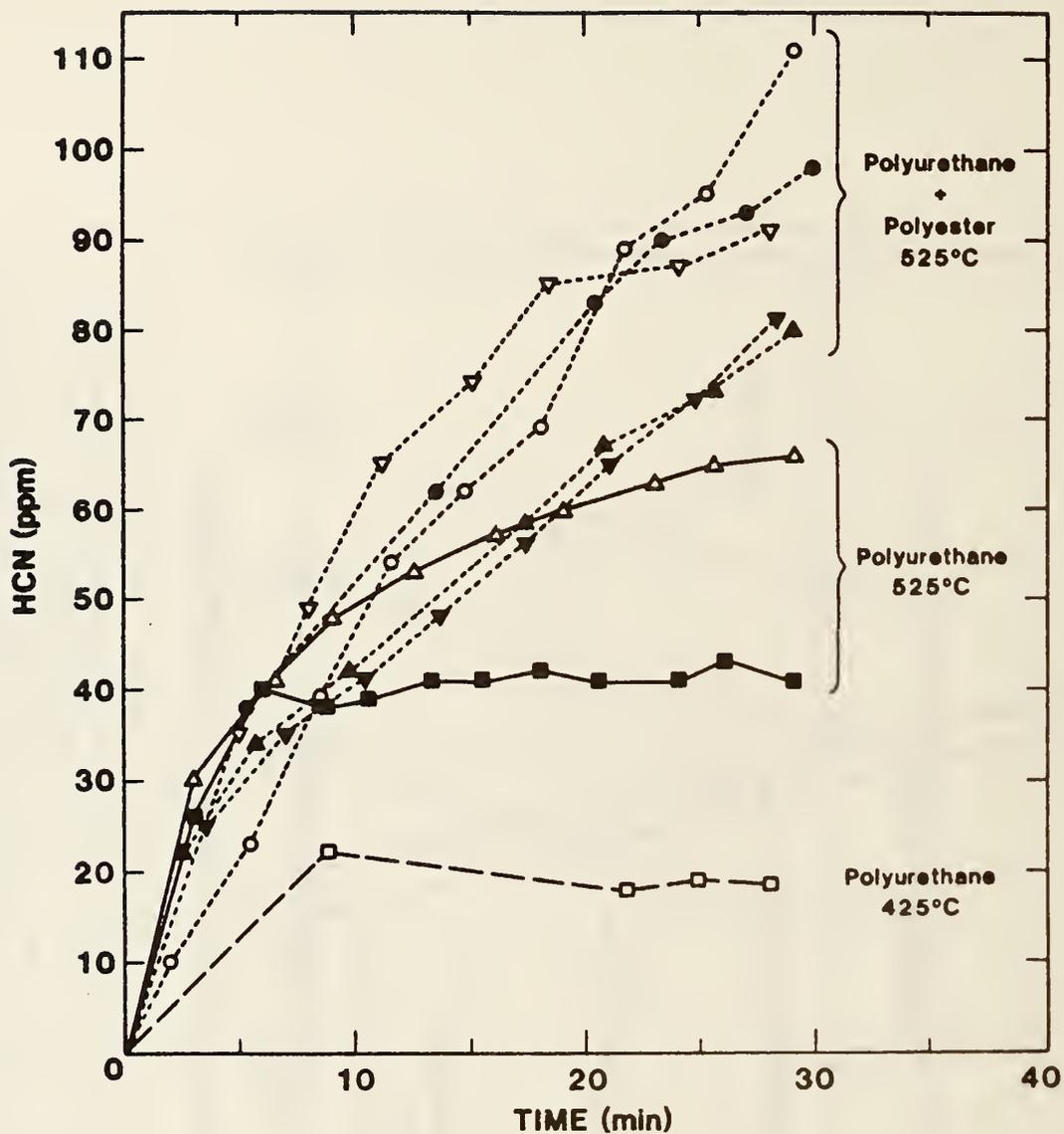


Figure 11. Generation of hydrogen cyanide from polyurethane decomposed in the flaming mode in the NBS toxicity test apparatus. In all cases, the mass loading of polyurethane was 3.88 g (20 mg/l). Polyurethane decomposed alone at 425°C (□-□) or at 525°C (■-■, Δ-Δ); 20 mg/l polyurethane at 525°C with polyester at 22.5 mg/l (▲), 25 mg/l (▼), 15 mg/l (▽), 20 mg/l (●), 30 mg/l (○).....

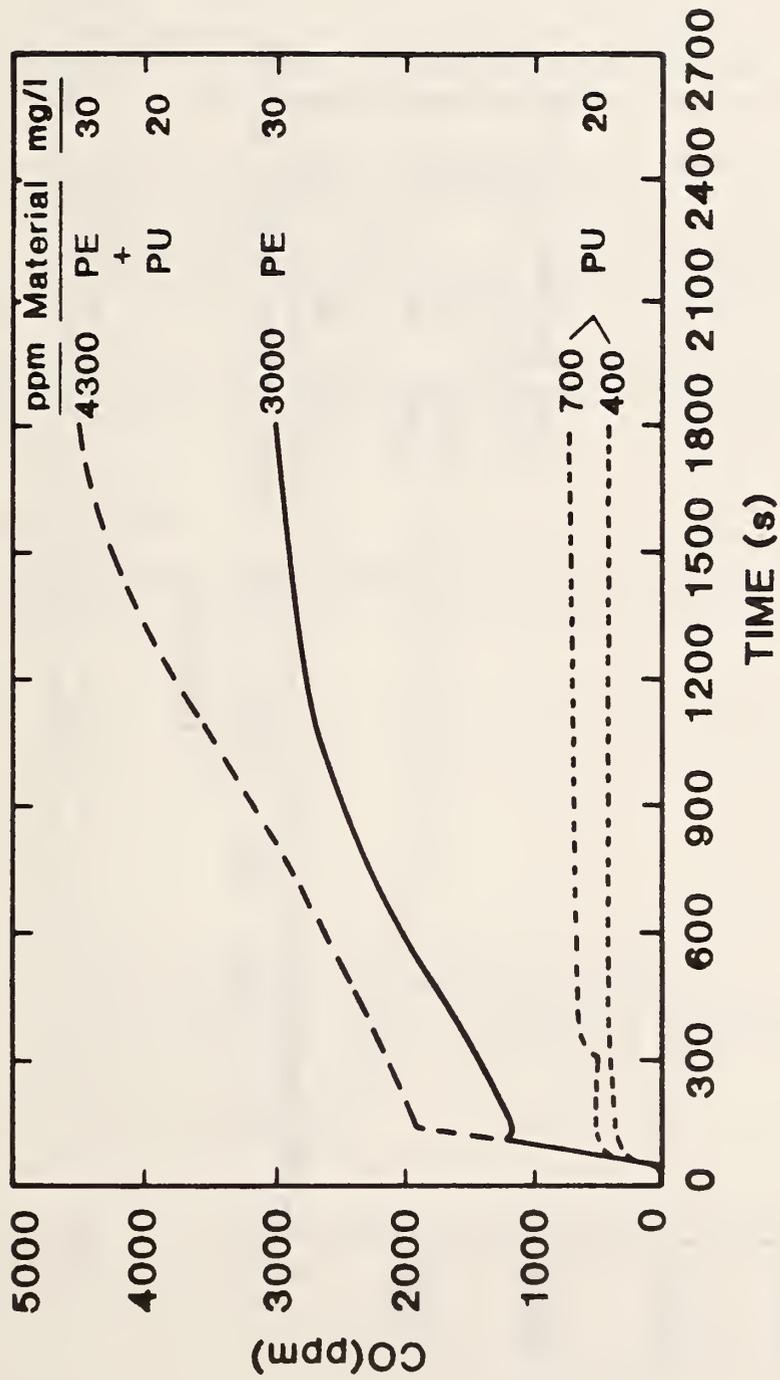


Figure 12. CO generation from flexible polyurethane foam and polyester decomposed along and together. (Flaming, 525°C, NBS Toxicity Test Method)

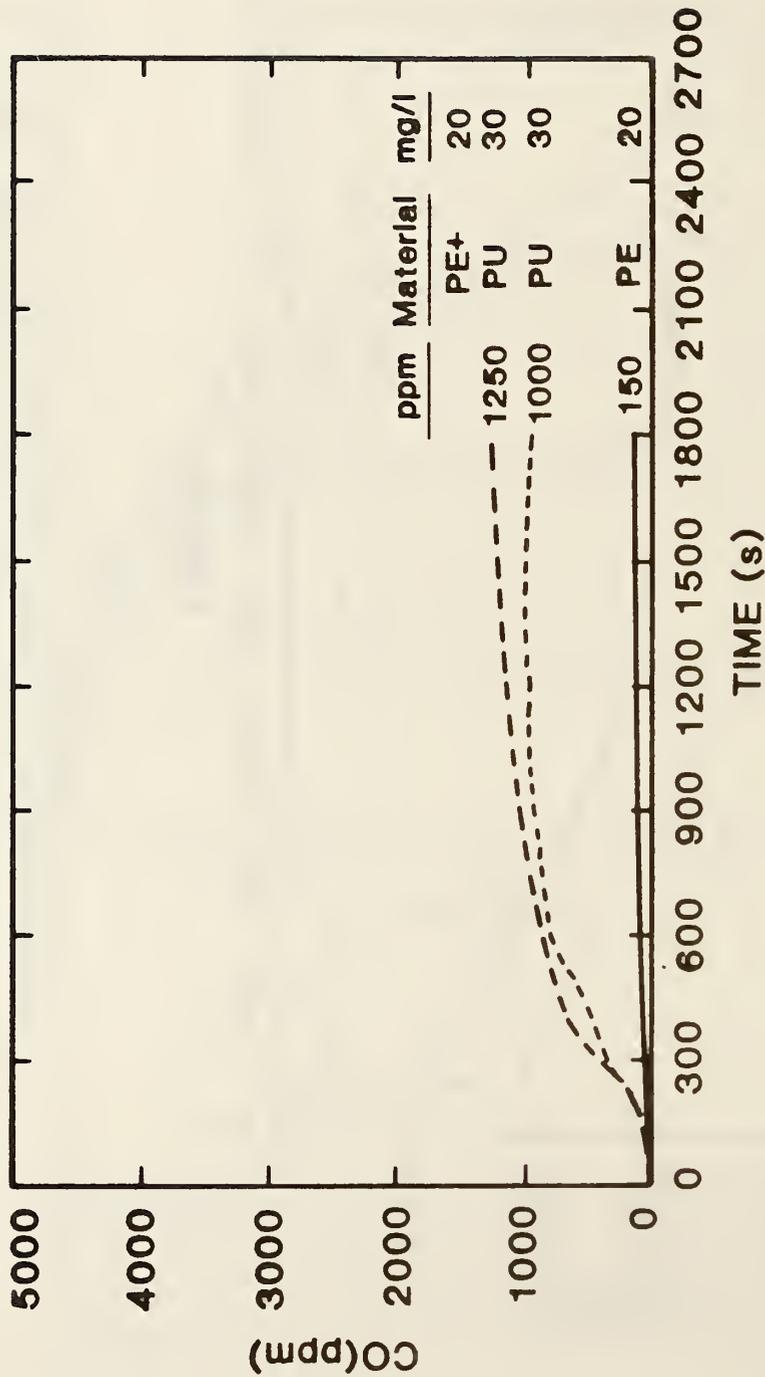


Figure 13. CO generation from flexible polyurethane foam and polyester decomposed alone and together. (Non-flaming, 375°C, NBS Toxicity Test Method)

## APPENDIX A

The derivation of the equation describing the material concentration in the animal exposure chamber assumes that:

- the pyrolysate generated in the combustion chamber is instantaneously mixed throughout the volume of the combustion chamber. This is an approximation of experimental observations;
- the pyrolysate concentration is not altered by loss of material to the interior surfaces of the combustion chamber, exhaust duct, connecting pipe, and animal exposure chamber. This is also an approximation, since soot and tar deposits were observed in the connecting pipe and control valve located between the exhaust duct and the animal exposure chamber.

The problem is divided into two parts. First, a solution is developed for the material concentration in the combustion chamber. Second, an equation is developed that describes the filling process of the exposure chamber from the combustion chamber.

### I. Combustion Chamber

The change of pyrolysate in the combustion chamber is given by:

$$\frac{dC_b}{dt} = \frac{f(t)}{V_b} - \frac{\dot{v}_o}{V_b} C_b \quad (1)$$

where

$C_b$	=	the pyrolysate concentration, mg/l
$V_b$	=	the volume of the combustion chamber, l
$\dot{v}_o$	=	the volumetric airflow through the combustion chamber, l/s
$f(t)$	=	the generation rate of pyrolysate, mg/s

rewriting equation (1) as,

$$\frac{dC_b}{dt} + \frac{\dot{v}_o}{V_b} C_b = \frac{f(t)}{V_b} \quad (2)$$

one can solve this first order ordinary differential equation by multiplying by  $\exp(\dot{v}_o t/V_b)$ . This leads to a solution of equations of the form,

$$C_b = \exp\left(-\frac{\dot{v}_o}{V_b} t\right) \int \exp\left(\frac{\dot{v}_o}{V_b} t\right) \frac{f(t)}{V_b} dt + D \exp\left(-\frac{\dot{v}_o}{V_b} t\right) \quad (3)$$

where  $D$  = an arbitrary constant determined by initial conditions.

For a given function of  $f(t)$ , the problem of determining a solution of equation (2) is reduced to that of evaluating the antiderivative in equation (3) and the application of initial conditions. Since the actual calculations that were performed assumed constant mass loss rate, equation (2) will be solved for  $f(t) = \dot{m}$ , constant, using two different initial conditions, at time  $t = 0$  and either  $C_b = 0$  or  $C_b = K_1$ . Where  $K_1$  is some initial concentration in the exposure chamber.

For  $f(t) = \dot{m}$

Substituting  $\dot{m}$  for  $f(t)$  in equation (3), the integral

$$\int \exp\left(\frac{\dot{v}_o}{V_b} t\right) \frac{f(t)}{V_b} dt = \int \exp\left(\frac{\dot{v}_o}{V_b} t\right) \frac{\dot{m}}{V_b} dt \quad (4)$$

Moving constants out of the integral and performing the integration yields

$$\frac{\dot{m}}{V_b} \int \exp\left(\frac{\dot{v}_o}{V_b} t\right) dt = \frac{\dot{m}}{V_b} \frac{V_b}{\dot{v}_o} \exp\left(\frac{\dot{v}_o}{V_b} t\right) = \frac{\dot{m}}{\dot{v}_o} \exp\left(\frac{\dot{v}_o}{V_b} t\right) \quad (5)$$

Equation (5) is substituted for the integral in equation (3). Rearranging terms yields

$$C_b = \frac{\dot{m}}{\dot{v}_o} + D \exp\left(-\frac{\dot{v}_o}{V_b} t\right) \quad (6)$$

For initial conditions  $t = 0, C_b = 0$

Applying initial conditions yields a value for the arbitrary constant of

$$D = -\frac{\dot{m}}{\dot{v}_o} \quad (7)$$

Substituting equation (7) into equation (6) produces an exact solution for the concentration of pyrolysate in the combustion chamber.

$$C_b = \frac{\dot{m}}{\dot{v}_o} \left(1 - \exp\left(-\frac{\dot{v}_o}{V_b} t\right)\right) \quad (8)$$

For initial conditions  $t = 0, C_b = K_1$

Applying these initial conditions to equation (6) yields a different value for the arbitrary constant of

$$D = K_1 - \frac{\dot{m}}{\dot{v}_o} \quad (9)$$

Substituting equation (9) into equation (6) produces the following exact solution

$$C_b = \frac{\dot{m}}{\dot{v}_o} (1 - \exp(-\frac{\dot{v}_o}{V_b} t)) + K_1 \exp(-\frac{\dot{v}_o}{V_b} t) \quad (10)$$

## II. Exposure Chamber Concentration

It was assumed that the animal exposure chamber was being filled at the material concentration calculated for the combustion chamber. The change in the concentration in the exposure chamber is then given by

$$\frac{dC_e}{dt} = \frac{g(t)}{V_e} C_b \quad (11)$$

where

- $C_e$  = the pyrolysate concentration in the exposure chamber, mg/l
- $V_e$  = the volume of the animal exposure chamber, l
- $g(t)$  = the volumetric flow rate between combustion chamber and exposure chamber, l/s

Solving for the animal exposure chamber concentration yields

$$C_e = \int_0^{t_1} \frac{g(t)}{V_e} C_b dt \quad (12)$$

If  $g(t)$  and  $V_e$  are constants, as they were in these experiments, equation (12) is solved by substituting either equation (8) or (10) for  $C_b$  and performing the integration from  $t = 0$ , the start of exposure chamber filling to  $t = t_1$ , the end of the filling process:

$$C_e = \frac{G}{V_e} \int_0^{t_1} C_b dt \quad (13)$$

where  $G = g(t)$ , a constant filling rate,  $l/s$

Using equation (10) with equation (13),

$$C_e = \frac{G}{V_e} \int_0^{t_1} \left[ \frac{\dot{m}}{\dot{v}_o} (1 - \exp(-\frac{\dot{v}_o}{V_b} t)) + K_1 \exp(-\frac{\dot{v}_o}{V_b} t) \right] dt \quad (14)$$

After performing the integration, this simplifies to

$$C_e = \frac{G}{V_e \dot{v}_o} \left[ \dot{m} t_1 + (1 - \exp(-\frac{\dot{v}_o}{V_b} t_1)) (K_1 V_b - \dot{m} \frac{V_b}{\dot{v}_o}) \right] \quad (15)$$

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<b>5. AUTHOR(S)</b> Barbara C. Levin, Emil Braun, Joshua L. Gurman, Maya Paabo			
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<b>9. SPONSORING ORGANIZATION NAME AND COMPLETE ADDRESS</b> <i>(Street, City, State, ZIP)</i>  U. S. Consumer Product Safety Commission Bethesda, MD 20207			
<b>10. SUPPLEMENTARY NOTES</b>  <input type="checkbox"/> Document describes a computer program; SF-185, FIPS Software Summary, is attached.			
<b>11. ABSTRACT</b> <i>(A 200-word or less factual summary of most significant information. If document includes a significant bibliography or literature survey, mention it here)</i> Representative specimens of flexible polyurethane foam and polyester fabric were thermally decomposed separately and together in order to compare the toxicity of the combustion products from the combined materials with those from the single homogeneous materials and to compare the toxicological results obtained with the NBS Toxicity Test Method with those using a cone radiant heater toxicity test apparatus. Gas concentrations (CO, CO <sub>2</sub> , O <sub>2</sub> and HCN), blood carboxyhemoglobin, and LC <sub>50</sub> values in Fischer 344 rats were determined for the materials under both flaming and non-flaming conditions. With the NBS Toxicity Test Method, the results of the non-flaming combined experiments indicated that both materials contributed in an additive manner to the concentration of the combustion products. However, under flaming conditions, the generation of HCN is greater than that predicted from the addition of the maximum amounts produced by the materials separately. With the cone radiant heater under conditions designed to generate the maximum concentrations of combustion products, animal deaths were observed in the combination experiments, but not in the single material exposures. In the combined material testing with both toxicity test systems, flaming conditions produced deaths during the 30 minute exposures; whereas, non-flaming conditions produced deaths following the exposures. Estimated LC <sub>50</sub> values for the combined materials in the radiant furnace were not greatly different from the calculated values obtained with the NBS Toxicity Test.			
<b>12. KEY WORDS</b> <i>(Six to twelve entries; alphabetical order; capitalize only proper names; and separate key words by semicolons)</i> combustion products; inhalation; lethal concentrations; Toxicity Test Methods; polyesters; polyurethane foams; radiant heat; toxicity; upholstered furniture.			
<b>13. AVAILABILITY</b> <input checked="" type="checkbox"/> Unlimited <input type="checkbox"/> For Official Distribution. Do Not Release to NTIS <input type="checkbox"/> Order From Superintendent of Documents, U.S. Government Printing Office, Washington, DC 20402. <input checked="" type="checkbox"/> Order From National Technical Information Service (NTIS), Springfield, VA 22161		<b>14. NO. OF PRINTED PAGES</b>  70	<b>15. Price</b>  \$11.95



